

## Supplementary Information for

### The synergy between Fe and Ni in the Optimal Performance of (Ni,Fe)OOH Catalysts for the Oxygen Evolution Reaction

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References for SI reference citations

## Supporting Information Text

### I. Methods

**Structure optimization with PBE.** The optimization of structures was performed with the VASP package (1–3), using the PBE flavor (4) of DFT including the D3 London Dispersion correction. We used the projector augmented wave (PAW) method (5) to account for core-valence interactions. The kinetic energy cutoff for plane wave expansions was set to 400 eV, and reciprocal space was sampled by the  $\Gamma$ -centered Monkhorst-Pack scheme with a grid of  $3 \times 3 \times 1$  for surface calculations. The convergence criteria are  $1 \times 10^{-5}$  and  $1 \times 10^{-7}$  eV energy differences for solving for the electronic wave function for local minima and transition states (TS), respectively. All atomic coordinates are converged to within  $3 \times 10^{-2}$  eV/Å for maximal components of forces. The TS search was conducted by using the climbing image nudged elastic band (CI-NEB) method (6) to generate initial guess geometries, followed by the dimer method (7) to converge to the saddle points. The phonon contributions to the zero-point energies (ZPE), enthalpy, and entropy were included in calculating the free energies at room temperature (298.15 K) as in our previous work (8, 9).

**Energy calculations with B3PW91.** The hybrid functional B3PW91 calculations were performed using the CRYSTAL14 package (10), which uses local atomic Gaussian-type basis sets. This enables fast evaluation of the Hartree-Fock exchange terms required for the hybrid functional method. We used the all-electron 6-311G(d) basis sets of triple- $\zeta$  quality for H, O and K (11), while for Ni and Fe, we used the SBKJC relativistic effective core potentials with associated basis sets modified to triple- $\zeta$  quality (12). An extra-large grid, consisting of 75 radial points and 974 angular points, was used for accurate integration. All other settings are similar to those in VASP calculations.

**Grand Canonical QM calculations with PBE.** Rather than the normal QM in which the number of electrons are kept fixed, we carried out Grand Canonical QM in which the chemical potential ( $\mu_e$ ) is constant. Our GC-QM method uses the implicit CANDLE solvation model (13) as performed using JDFTx (14). The GBRV ultrasoft pseudopotentials (15) were used, with a plane wave cutoff of 544 eV (20 au). All other settings are similar to those standard in VASP calculations. The ionic screening of net charges resulting from the constant  $\mu_e$  condition was achieved with cation (0.1 M  $K^+$ ) and anion (0.1 M  $F^-$ ) components in the fluid model (16) under the JDFT framework (17). The algorithm employed by JDFTx variationally minimizes the grand free energy at fixed electron chemical potential with respect to Kohn-Sham orbitals (18), fluid bound charge, and an auxiliary Hamiltonian for the occupations (19). Previously, we found that the relative free energies (including barriers) are linearly dependent on  $U$  for  $|U| < \sim 2$  V (8), so we calculated the  $U$ -dependence assuming a linear relationship between  $U = 0.0$  and  $+1.9$  V.

**Effects of electrolyte properties.** The pH effect was included through the chemical potential of  $H^+$  by referencing to the standard hydrogen electrode reaction  $H^+ + e^- = \frac{1}{2}H_2$ , as in our previous work (8, 9). This scheme naturally covers the thermochemistry of pH-dependent states throughout the OER mechanisms, such as the surface states dictated by the Pourbaix diagram (20). However, for calculating the overpotentials, the pH term is canceled by taking the difference between predicted onset potentials and the equilibrium OER potential, so we do not discuss pH effects.

The implicit CANDLE solvation model (13) used here includes the charge screening effect of both ions in the electrolyte, but it does not account for anions explicitly. Anions have been shown to serve as the proton acceptor so that they affect the kinetics at very low concentrations ( $< 0.03$  M), but enable fast deprotonation associated with the electrochemical oxidation at larger concentrations (21). This is consistent with our assumption, based on which we ignored the kinetics of deprotonation in our calculations (with 0.1 M anion). Although borate anions have been shown to inhibit the O-O coupling in OER for the Co-OEC complex which involves the IMOC mechanism (22), we did not consider such specific effect in our studies.

**Microkinetic model.** We assumed that OER elementary steps that are simple deprotonation process associated with electrochemical oxidation have very fast kinetics, reaching thermodynamic equilibrium instantaneously. Because the largest free energy input required is for either the 1e step or the O radical formation step, both of which are before the O-O coupling, we assumed that the states before the O-O coupling dominate the catalyst surfaces. According to the Boltzmann distribution, the ratios among the states can be determined with the  $U$ -dependent free energy differences by adding the electrochemical  $eU$  energy contribution. Thus the surface concentration of O radical  $C[*O\bullet]$  can be expressed as a function of  $U$ , and the O-O coupling reaction rate  $r = k \cdot C[*O\bullet]$ , where the rate constant  $k = A \cdot \exp(-\Delta G^\ddagger/k_B T)$  and  $A = k_B T/h$ , based on transition state theory. Note that the free energy barrier  $\Delta G^\ddagger$  is also  $U$ -dependent. Then, the current density is expressed as  $j = n_e C_e \cdot r$ , where  $n_e$  is the number of electrons transferred, and  $C_e$  is the elementary charge. Finally, we numerically solve for the  $U$  that corresponds to  $j = 10$  mA/cm<sup>2</sup>.

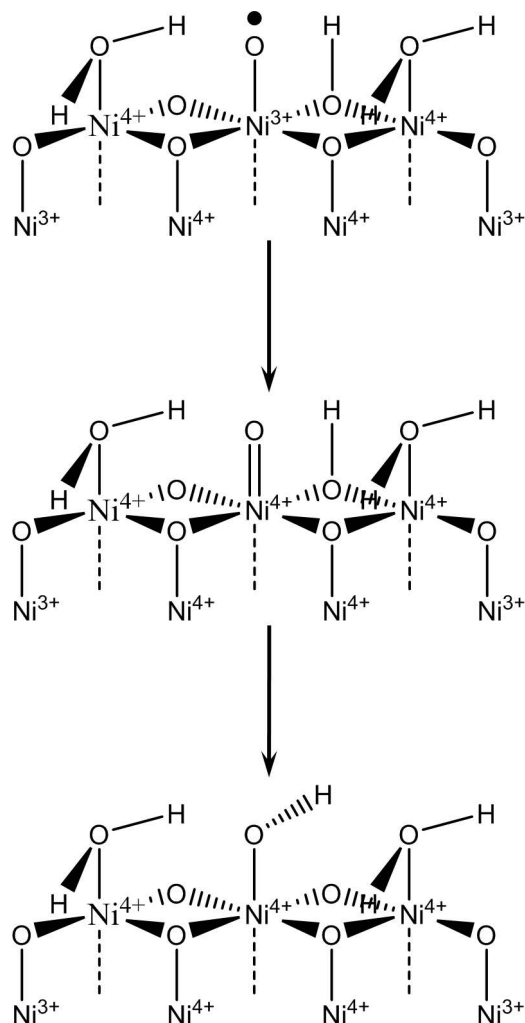
### II. Additional discussions

**Fe doping in NiOOH.** Since all Ni sites in bulk  $\beta$ -NiOOH are equivalent by symmetry (all are  $Ni^{3+}$  sites), we do not need to consider the preferential location of Fe substitution in bulk  $\beta$ -NiOOH. As for the  $\beta$ -NiOOH surface, we found a similar trend that Fe favors the surface site over the subsurface site by 0.1 eV.

In the  $\gamma$ -NiOOH system, we showed that Fe substitution favors the  $Ni^{4+}$  site over  $Ni^{3+}$  site, consistent with Ref. (23), which has shown that when the  $\beta$ -phase is transformed into  $\gamma$ -phase, Fe is oxidized to +4 before Ni.

We refer the readers to Ref. (23) for the energies associated with the formation of  $\text{Fe}^{4+}$  from  $\text{Fe}^{3+}$  accompanying the bulk phase transformation from the  $\beta$ -phase to the  $\gamma$ -phase.

**The possible alternative pathway through  $\text{Ni(III)-O}\cdot$ .**  $\text{Ni(III)-O}\cdot$  is thermodynamically unstable, higher in energy by 0.2 eV than its resonance state  $\text{Ni(IV)=O}$ , which converts to  $\text{Ni(IV)-OH}$  (energy further going down by 0.6 eV) by taking the proton from the neighboring bridging O (this is the State 2 in Figure 2), as shown below.



At very high pH, the bridging OH ( $\mu\text{-OH}$ ) is deprotonated to  $\mu\text{-O}^-$ , so that then it is  $\mu\text{-O}^-$  that transfers its charge to  $\text{Ni(IV)=O}$  to produce  $\text{Ni(IV)-O}^-$ .

It is only after State 3 in Figure 2 (with all surface Ni oxidized to  $\text{Ni}^{4+}$ ) that the O radical ( $\text{Ni(IV)-O}\cdot$ ) is the most stable configuration, and it cannot resonate into  $\text{Ni(V)=O}$ .

**The possible alternative pathway through  $\text{Fe(III)-O}\cdot$ .** Fe is present as  $\text{Fe}^{4+}$  in the OER active  $\gamma$ -phase, so We do not consider  $\text{Fe(III)-O}\cdot$  since it would require first reduction of  $\text{Fe(IV)}$  to  $\text{Fe(III)}$  under an oxidative environment, and even if this could happen (by oxidizing  $\text{Ni(III)}$  to  $\text{Ni(IV)}$  internally as  $\text{Fe(IV)} + \text{Ni(III)} = \text{Fe(III)} + \text{Ni(IV)}$ ), it would cost 0.5 eV, so we expect that  $\text{Fe(III)}$  is unstable during OER.

### III. Structural information: coordinates for all predicted intermediates and transition states

Figure 2a State 1

```
1.0000000000000000
8.7372206091223994    0.0000000000000000    0.0000000000000000
0.0000000000000000    6.9809029500783426    0.0000000000000000
0.0000000000000000    0.0000000000000000    25.0000000000000000
K      Ni      O      H
4      12      34      20
```

# Selective dynamics

## Direct

0.0000000000000000	0.9295476953180497	0.0219900692777486	F	F	F
0.5000000000000000	0.8431778700801544	0.1149178963106294	F	F	F
0.0476265895605332	0.7587938012328159	0.2091379063941224	T	T	T
0.5446401208633082	0.6881690734822580	0.3413329835919385	T	T	T
0.0000000000000000	0.4295476953180497	0.0219900692777486	F	F	F
0.3336660000000000	0.4295476953180497	0.0219900692777486	F	F	F
0.6663339999999991	0.4295476953180497	0.0219900692777486	F	F	F
0.1663339999999991	0.3431778700801544	0.1149178963106294	F	F	F
0.5000000000000000	0.3431778700801544	0.1149178963106294	F	F	F
0.8336660000000000	0.3431778700801544	0.1149178963106294	F	F	F
0.0005345777564151	0.2557512551908413	0.2098658176066714	T	T	T
0.3329281744243836	0.2541498356372988	0.2097975444809000	T	T	T
0.6640616948871436	0.2537483352104428	0.2100935898948935	T	T	T
0.1643546527638344	0.1759128747991577	0.3056366004034719	T	T	T
0.5056079199153924	0.1754622428115751	0.3055546964321286	T	T	T
0.8338015032706425	0.1865395973448115	0.3069785268400112	T	T	T
0.1735150000000019	0.5955569454815901	0.0004884286588833	F	F	F
0.5000000000000000	0.5859389052830437	0.0000000000000000	F	F	F
0.8264849999999981	0.5955569454815901	0.0004884286588833	F	F	F
0.1735150000000019	0.2635384451545022	0.0434917098966210	F	F	F
0.5000000000000000	0.2731564853530557	0.0439801385555043	F	F	F
0.8264849999999981	0.2635384451545022	0.0434917098966210	F	F	F
0.0000000000000000	0.4995690800451484	0.0929278270328737	F	F	F
0.3264849999999981	0.5091871202437019	0.0934162556917641	F	F	F
0.6735150000000019	0.5091871202437019	0.0934162556917641	F	F	F
0.0000000000000000	0.1867866601151604	0.1369079655883780	F	F	F
0.3264849999999981	0.1771686199166140	0.1364195369294947	F	F	F
0.6735150000000019	0.1771686199166140	0.1364195369294947	F	F	F
0.1715937907011299	0.4171740334167923	0.1875477333914071	T	T	T
0.4988713303020128	0.4154238985146965	0.1876130063360404	T	T	T
0.8297878923126433	0.4159566401250225	0.1889595921826081	T	T	T
0.1698836363977670	0.0969476392984761	0.2327611001496789	T	T	T
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0.8229795892288464	0.0941970708305794	0.2358447497236240	T	T	T
0.0043315940096047	0.3345371981586341	0.2806696771574873	T	T	T
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0.3378181117622844	0.0227526893815597	0.3321799250900476	T	T	T
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0.1563629999999989	0.8431778700801544	0.1149178963106294	F	F	F
0.8436370000000011	0.8431778700801544	0.1149178963106294	F	F	F
0.3643749309520727	0.7274533950051004	0.2464557194064731	T	T	T
0.7495669497512880	0.7214804422987457	0.2568605233610383	T	T	T
0.2215754710200228	0.6385645614950288	0.3530898131014557	T	T	T
0.8882372592748637	0.6896182727369018	0.3542412378336434	T	T	T
0.8668731788582661	0.3041400617570768	0.3773410876892010	T	T	T
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0.7222089999999994	0.8194148176612188	0.0136009167645312	F	F	F
0.7222089999999994	0.0396805729748735	0.0303792217909731	F	F	F
0.2222089999999994	0.7330449924233307	0.1065287437974050	F	F	F
0.2222089999999994	0.9533107477369782	0.1233070488238468	F	F	F
0.7777910000000006	0.7330449924233307	0.1065287437974050	F	F	F
0.7777910000000006	0.9533107477369782	0.1233070488238468	F	F	F
0.4187284233679572	0.6257997704471786	0.2266522930595830	T	T	T

0.4167858152080779	0.8501260697103067	0.2388459274896567	T	T	T
0.7612374986571477	0.6273135622861563	0.2276588821074240	T	T	T
0.7638677888050497	0.8544876016861330	0.2433796079807767	T	T	T
0.2485274512311111	0.6536007041212080	0.3150593210640724	T	T	T
0.1121697789266454	0.6730665099497096	0.3548556569556258	T	T	T
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0.3184470517897417	0.0619888927826935	0.3695827776145412	T	T	T
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Figure 2a State 2

1.000000000000000		
8.7372206091223994	0.0000000000000000	0.0000000000000000
0.0000000000000000	6.9809029500783426	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000

K	Ni	O	H
4	12	35	21

Selective dynamics

Direct

0.0000000000000000	0.9295476953180497	0.0219900692777486	F	F	F
0.5000000000000000	0.8431778700801544	0.1149178963106294	F	F	F
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0.5209184111331686	0.7054103600691909	0.3568705344811053	T	T	T
0.0000000000000000	0.4295476953180497	0.0219900692777486	F	F	F
0.3336660000000009	0.4295476953180497	0.0219900692777486	F	F	F
0.6663339999999991	0.4295476953180497	0.0219900692777486	F	F	F
0.1663339999999991	0.3431778700801544	0.1149178963106294	F	F	F
0.5000000000000000	0.3431778700801544	0.1149178963106294	F	F	F
0.8336660000000009	0.3431778700801544	0.1149178963106294	F	F	F
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0.6669847390604924	0.2566933251857333	0.2093612247731984	T	T	T
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0.5044588784796660	0.1846453575819847	0.3045421415531295	T	T	T
0.8337711046665753	0.1846524778465518	0.3046226619427934	T	T	T
0.1735150000000019	0.5955569454815901	0.0004884286588833	F	F	F
0.5000000000000000	0.5859389052830437	0.0000000000000000	F	F	F
0.8264849999999981	0.5955569454815901	0.0004884286588833	F	F	F
0.1735150000000019	0.2635384451545022	0.0434917098966210	F	F	F
0.5000000000000000	0.2731564853530557	0.0439801385555043	F	F	F
0.8264849999999981	0.2635384451545022	0.0434917098966210	F	F	F
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0.3436370000000011	0.9295476953180497	0.0219900692777486	F	F	F
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0.1563629999999989	0.8431778700801544	0.1149178963106294	F	F	F
0.8436370000000011	0.8431778700801544	0.1149178963106294	F	F	F
0.2875717602208159	0.7245308295909836	0.2668058636558665	T	T	T
0.7138135764823583	0.7145192607727716	0.2612556195697173	T	T	T
0.1802790295872390	0.6217130004622010	0.3623543067427505	T	T	T
0.8658905404616392	0.6956781973447472	0.3555426684608884	T	T	T
0.5172812475790859	0.3047326703434380	0.3724037613077616	T	T	T
0.8162915450201751	0.3034531089632375	0.3772491017077972	T	T	T
0.1683721338407403	0.2703788345013781	0.3783279643931243	T	T	T
0.2777910000000006	0.8194148176612188	0.0136009167645312	F	F	F
0.2777910000000006	0.0396805729748735	0.0303792217909731	F	F	F
0.7222089999999994	0.8194148176612188	0.0136009167645312	F	F	F
0.7222089999999994	0.0396805729748735	0.0303792217909731	F	F	F
0.2222089999999994	0.7330449924233307	0.1065287437974050	F	F	F
0.2222089999999994	0.9533107477369782	0.1233070488238468	F	F	F
0.7777910000000006	0.7330449924233307	0.1065287437974050	F	F	F
0.7777910000000006	0.9533107477369782	0.1233070488238468	F	F	F
0.3692291456602724	0.6534874693591984	0.2490823052028810	T	T	T
0.3247025914494318	0.8547934391384285	0.2794802235840514	T	T	T
0.7268057227187610	0.6304810723940066	0.2301280501450646	T	T	T
0.7139335433822435	0.8503092228503373	0.2508528340306402	T	T	T
0.2173115586898007	0.6416765686336885	0.3243965735741287	T	T	T
0.0707760453237117	0.6594100184456657	0.3607646469044217	T	T	T
0.8260410995607567	0.6880712561940233	0.3179931491813358	T	T	T
0.9009219876083446	0.8317806273625192	0.3569819097382507	T	T	T
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0.4400328698112133	0.2376866544639281	0.3937188307677165	T	T	T
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0.8375833884243584	0.4427781937513932	0.3734053402994115	T	T	T
0.1710281975306546	0.4233307894127077	0.3732312789072550	T	T	T

Figure 2a State 3

1.0000000000000000		
8.7372206091223994	0.0000000000000000	0.0000000000000000
0.0000000000000000	6.9809029500783426	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000

K    Ni    O    H  
4    12    35    20

Selective dynamics

Direct

0.0000000000000000	0.9295476953180497	0.0219900692777486	F	F	F
0.5000000000000000	0.8431778700801544	0.1149178963106294	F	F	F
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0.4922396351329520	0.7631739823774661	0.3856996442457001	T	T	T
0.0000000000000000	0.4295476953180497	0.0219900692777486	F	F	F
0.3336660000000009	0.4295476953180497	0.0219900692777486	F	F	F
0.6663339999999991	0.4295476953180497	0.0219900692777486	F	F	F
0.1663339999999991	0.3431778700801544	0.1149178963106294	F	F	F
0.5000000000000000	0.3431778700801544	0.1149178963106294	F	F	F
0.8336660000000009	0.3431778700801544	0.1149178963106294	F	F	F
0.9997170602402035	0.2664984532757443	0.2105615439411896	T	T	T
0.3319067280826627	0.2623866335574890	0.2095118744534370	T	T	T
0.6670387371555830	0.2621738132180873	0.2094197454237923	T	T	T
0.1663615711003474	0.1924758880668039	0.3063704177075092	T	T	T
0.4991536547297251	0.1963876195717008	0.3041763523765875	T	T	T
0.8315218754680557	0.1941142269630383	0.3059419855266546	T	T	T
0.1735150000000019	0.5955569454815901	0.0004884286588833	F	F	F
0.5000000000000000	0.5859389052830437	0.0000000000000000	F	F	F
0.8264849999999981	0.5955569454815901	0.0004884286588833	F	F	F

0.17351500000000019	0.2635384451545022	0.0434917098966210	F	F	F
0.50000000000000000	0.2731564853530557	0.0439801385555043	F	F	F
0.82648499999999981	0.2635384451545022	0.0434917098966210	F	F	F
0.00000000000000000	0.4995690800451484	0.0929278270328737	F	F	F
0.32648499999999981	0.5091871202437019	0.0934162556917641	F	F	F
0.67351500000000019	0.5091871202437019	0.0934162556917641	F	F	F
0.00000000000000000	0.1867866601151604	0.1369079655883780	F	F	F
0.32648499999999981	0.1771686199166140	0.1364195369294947	F	F	F
0.67351500000000019	0.1771686199166140	0.1364195369294947	F	F	F
0.1655806501996181	0.4214792501407900	0.1868477124647750	T	T	T
0.5000364121226522	0.4174224683830816	0.1863700872880935	T	T	T
0.8330560544691290	0.4216767757322997	0.1868097364715699	T	T	T
0.1646465068789108	0.1114497282866507	0.2333176944408555	T	T	T
0.4995842849613227	0.1065045407537052	0.2316277172135279	T	T	T
0.8353452552230608	0.1108334480965919	0.2341075344016525	T	T	T
0.9989665019396240	0.3500095678532818	0.2823901907207503	T	T	T
0.3335399732604090	0.3512326129506577	0.2800246471154212	T	T	T
0.6642979375195722	0.3524291606775042	0.2796404281453540	T	T	T
0.9991628151477863	0.0414199452430070	0.3239005348840882	T	T	T
0.3379349885764401	0.0370084074927560	0.3224453545779868	T	T	T
0.6613556122326991	0.0371879401244236	0.3223549816376129	T	T	T
0.34363700000000011	0.9295476953180497	0.0219900692777486	F	F	F
0.65636299999999989	0.9295476953180497	0.0219900692777486	F	F	F
0.15636299999999989	0.8431778700801544	0.1149178963106294	F	F	F
0.84363700000000011	0.8431778700801544	0.1149178963106294	F	F	F
0.2322797344468659	0.7170286713790519	0.2823049584077849	T	T	T
0.7665131234799664	0.7167316197607485	0.2844945545550980	T	T	T
0.1700303158695030	0.6654942055181909	0.3898806404931979	T	T	T
0.8552359512234774	0.6474199943010208	0.3849645587831911	T	T	T
0.5009577443803171	0.3133191287484285	0.3713984305325463	T	T	T
0.8116352020928402	0.2915954572119420	0.3776097764513502	T	T	T
0.1728224073116699	0.2841959028313581	0.3761226540824560	T	T	T
0.27779100000000006	0.8194148176612188	0.0136009167645312	F	F	F
0.27779100000000006	0.0396805729748735	0.0303792217909731	F	F	F
0.72220899999999994	0.8194148176612188	0.0136009167645312	F	F	F
0.72220899999999994	0.0396805729748735	0.0303792217909731	F	F	F
0.22220899999999994	0.7330449924233307	0.1065287437974050	F	F	F
0.22220899999999994	0.9533107477369782	0.1233070488238468	F	F	F
0.77779100000000006	0.7330449924233307	0.1065287437974050	F	F	F
0.77779100000000006	0.9533107477369782	0.1233070488238468	F	F	F
0.2964397353149535	0.6012420247833008	0.2786408389943860	T	T	T
0.2955437783480985	0.8350047115456903	0.2869665391649996	T	T	T
0.7010501119299205	0.6031385492866036	0.2787549947623301	T	T	T
0.7050304238171367	0.8368273024160158	0.2896624860752976	T	T	T
0.1757963550060604	0.7022210774605111	0.3513315068658710	T	T	T
0.1694478200187269	0.5217140051022540	0.3873180978002835	T	T	T
0.8376032416141318	0.6887972049031835	0.3468221837182724	T	T	T
0.9661713116866151	0.6745995496170023	0.3921341681203077	T	T	T
0.6981131953154738	0.2790618789422566	0.3836722212771377	T	T	T
0.3981080520738262	0.2796365218349357	0.3851955134843410	T	T	T
0.0900037548112964	0.2104731164762360	0.3928724713847497	T	T	T
0.8356629139625936	0.4415940549471409	0.3799603222448886	T	T	T

Figure 2a State 4

1.0000000000000000			
8.7372206091223994	0.0000000000000000	0.0000000000000000	
0.00000000000000000	6.9809029500783426	0.00000000000000000	
0.00000000000000000	0.0000000000000000	25.00000000000000000	
K	Ni	O	H
4	12	36	21

Selective dynamics



Direct					
0.0000000000000000	0.9295476953180497	0.0219900692777486	F	F	F
0.5000000000000000	0.8431778700801544	0.1149178963106294	F	F	F
0.9995436346577217	0.7648049790545549	0.2127874464375499	T	T	T
0.4812691444662215	0.8084739705931802	0.3995119048426438	T	T	T
0.0000000000000000	0.4295476953180497	0.0219900692777486	F	F	F
0.3336660000000009	0.4295476953180497	0.0219900692777486	F	F	F
0.6663339999999991	0.4295476953180497	0.0219900692777486	F	F	F
0.1663339999999991	0.3431778700801544	0.1149178963106294	F	F	F
0.5000000000000000	0.3431778700801544	0.1149178963106294	F	F	F
0.8336660000000009	0.3431778700801544	0.1149178963106294	F	F	F
0.0000660893534483	0.2645212479021420	0.2103168754565430	T	T	T
0.3323982022371466	0.2616677950885861	0.2098743301953655	T	T	T
0.6665576878151604	0.2604517505357838	0.2093429098104117	T	T	T
0.1656614767391175	0.1863148058806829	0.3062260542942715	T	T	T
0.5004663931775346	0.1937728562628641	0.3062189684890753	T	T	T
0.8324399466239766	0.1896190379566536	0.3052209659484209	T	T	T
0.1735150000000019	0.5955569454815901	0.0004884286588833	F	F	F
0.5000000000000000	0.5859389052830437	0.0000000000000000	F	F	F
0.8264849999999981	0.5955569454815901	0.0004884286588833	F	F	F
0.1735150000000019	0.2635384451545022	0.0434917098966210	F	F	F
0.5000000000000000	0.2731564853530557	0.0439801385555043	F	F	F
0.8264849999999981	0.2635384451545022	0.0434917098966210	F	F	F
0.0000000000000000	0.4995690800451484	0.0929278270328737	F	F	F
0.3264849999999981	0.5091871202437019	0.0934162556917641	F	F	F
0.6735150000000019	0.5091871202437019	0.0934162556917641	F	F	F
0.0000000000000000	0.1867866601151604	0.1369079655883780	F	F	F
0.3264849999999981	0.1771686199166140	0.1364195369294947	F	F	F
0.6735150000000019	0.1771686199166140	0.1364195369294947	F	F	F
0.1656142346719982	0.4208129563216241	0.1870282048268358	T	T	T
0.5001240301069215	0.4167597971908858	0.1866060235771633	T	T	T
0.8333416109608914	0.4203750703669852	0.1869416125589836	T	T	T
0.1658015954374450	0.1096911349248802	0.2329156344095602	T	T	T
0.4989571721445493	0.1061203271024126	0.2318291191814862	T	T	T
0.8348155372374532	0.1080094525440104	0.2331896757316794	T	T	T
0.9996927589026552	0.3453118372487349	0.2822680296788597	T	T	T
0.3331599846908714	0.3478447323739237	0.2809741376878463	T	T	T
0.6649933237043980	0.3486895499779599	0.2796149341486857	T	T	T
0.9979993418211818	0.0330231289839328	0.3219026706784769	T	T	T
0.3387620194195291	0.0334598189630827	0.3220889047911857	T	T	T
0.6632591418737112	0.0335711983606590	0.3229931299692285	T	T	T
0.3436370000000011	0.9295476953180497	0.0219900692777486	F	F	F
0.6563629999999989	0.9295476953180497	0.0219900692777486	F	F	F
0.1563629999999989	0.8431778700801544	0.1149178963106294	F	F	F
0.8436370000000011	0.8431778700801544	0.1149178963106294	F	F	F
0.2365277288951201	0.7129308152408536	0.2814385866897741	T	T	T
0.7666460301965556	0.7131458671356026	0.2851979630500604	T	T	T
0.1793533625562136	0.6539901310106296	0.3885856346012152	T	T	T
0.8668378367882724	0.6417922375320464	0.3847937917577255	T	T	T
0.5171004224595910	0.3135519696485981	0.3684073290747251	T	T	T
0.8169771232067899	0.2905757557980986	0.3762010997055383	T	T	T
0.1607807272853549	0.2682157677441492	0.3772413349270605	T	T	T
0.3563344642476712	0.1083372670214665	0.4476828447666104	T	T	T
0.2777910000000006	0.8194148176612188	0.0136009167645312	F	F	F
0.2777910000000006	0.0396805729748735	0.0303792217909731	F	F	F
0.7222089999999994	0.8194148176612188	0.0136009167645312	F	F	F
0.7222089999999994	0.0396805729748735	0.0303792217909731	F	F	F
0.2222089999999994	0.7330449924233307	0.1065287437974050	F	F	F
0.2222089999999994	0.9533107477369782	0.1233070488238468	F	F	F
0.7777910000000006	0.7330449924233307	0.1065287437974050	F	F	F
0.7777910000000006	0.9533107477369782	0.1233070488238468	F	F	F



0.3000464981126320	0.5960434271029657	0.2790258878919289	T	T	T
0.3011455170055853	0.8288334873487213	0.2868145574017614	T	T	T
0.7008366959709191	0.5992972694135941	0.2808002801722330	T	T	T
0.7039279834995816	0.8313760902583116	0.2914506843426020	T	T	T
0.1867540667777394	0.6893853589871939	0.3499348014577112	T	T	T
0.1793254244232708	0.5106793645808098	0.3866871688515241	T	T	T
0.8435563134488340	0.6869696612871822	0.3474242710994671	T	T	T
0.9790780158082532	0.6668620467578327	0.3904690559588850	T	T	T
0.7000841184585621	0.2838784509286342	0.3808384918485752	T	T	T
0.0611170526538252	0.2164285220555863	0.3886492042128687	T	T	T
0.8446983572723415	0.4420357494267718	0.3787325100197929	T	T	T
0.3783236239723713	0.2106107707719380	0.4728562073962904	T	T	T
0.2874854082484720	0.1672928146227628	0.4197231071069997	T	T	T

Figure 2a State 4 → 4' TS

1.0000000000000000		
8.7372206091223994	0.0000000000000000	0.0000000000000000
0.0000000000000000	6.9809029500783426	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000

K    Ni    O    H  
4   12   36   21  
Selective dynamics

Direct					
0.0000000000000000	0.9295476953180499	0.0219900692777486	F	F	F
0.5000000000000000	0.8431778700801544	0.1149178963106294	F	F	F
0.0014938095227780	0.7674262034237540	0.2119015700465292	T	T	T
0.5215121774700342	0.7455762120154146	0.4016210491823082	T	T	T
0.0000000000000000	0.4295476953180497	0.0219900692777486	F	F	F
0.3336660000000009	0.4295476953180497	0.0219900692777486	F	F	F
0.6663339999999991	0.4295476953180497	0.0219900692777486	F	F	F
0.1663339999999991	0.3431778700801546	0.1149178963106294	F	F	F
0.5000000000000000	0.3431778700801546	0.1149178963106294	F	F	F
0.8336660000000009	0.3431778700801546	0.1149178963106294	F	F	F
0.0002307520775367	0.2665361398157513	0.2101722115481535	T	T	T
0.3322004192230255	0.2637157677040273	0.2097675296247760	T	T	T
0.6668157974533270	0.2624336386096603	0.2091876079169103	T	T	T
0.1626435455610261	0.1959728448782997	0.3067766358537519	T	T	T
0.5036666910605115	0.1972570020260603	0.3041989497594798	T	T	T
0.8319615022913290	0.1940584106029367	0.3051072403644684	T	T	T
0.1735150000000019	0.5955569454815901	0.0004884286588833	F	F	F
0.5000000000000000	0.5859389052830437	0.0000000000000000	F	F	F
0.8264849999999981	0.5955569454815901	0.0004884286588833	F	F	F
0.1735150000000019	0.2635384451545022	0.0434917098966210	F	F	F
0.5000000000000000	0.2731564853530558	0.0439801385555043	F	F	F
0.8264849999999981	0.2635384451545022	0.0434917098966210	F	F	F
0.0000000000000000	0.4995690800451486	0.0929278270328737	F	F	F
0.3264849999999981	0.5091871202437019	0.0934162556917641	F	F	F
0.6735150000000019	0.5091871202437019	0.0934162556917641	F	F	F
0.0000000000000000	0.1867866601151605	0.1369079655883780	F	F	F
0.3264849999999981	0.1771686199166141	0.1364195369294947	F	F	F
0.6735150000000019	0.1771686199166141	0.1364195369294947	F	F	F
0.1656495973656807	0.4221463851453547	0.1869499316960922	T	T	T
0.5002070052604510	0.4177098461264794	0.1864032823625233	T	T	T
0.8337700286047939	0.4212634876068645	0.1869218359149478	T	T	T
0.1661302387644343	0.1123073329812640	0.2339929952854978	T	T	T
0.4983480851303374	0.1069366976754019	0.2314283955993683	T	T	T
0.8353459692724153	0.1105884186552970	0.2335326473459982	T	T	T
0.9998073969181741	0.3504474384647988	0.2820078800630139	T	T	T
0.3346063549704059	0.3522793169974479	0.2807616098539751	T	T	T
0.6642880481245560	0.3528188449737187	0.2798045988873789	T	T	T
0.9975566676568587	0.0409512222939640	0.3229313686880899	T	T	T

0.3385350128785333	0.0407348032202971	0.3264602304575094	T	T	T
0.6639736817203772	0.0357400298960868	0.3210126659121707	T	T	T
0.3436370000000011	0.9295476953180499	0.0219900692777486	F	F	F
0.6563629999999989	0.9295476953180499	0.0219900692777486	F	F	F
0.1563629999999989	0.8431778700801544	0.1149178963106294	F	F	F
0.8436370000000011	0.8431778700801544	0.1149178963106294	F	F	F
0.2322649278741634	0.7133412019769985	0.2841110949012908	T	T	T
0.7683334749050598	0.7153349854876296	0.2849736647300447	T	T	T
0.1852118080657829	0.6693799997528285	0.3932250982654770	T	T	T
0.8623086013184811	0.6529643463405616	0.3855696875345794	T	T	T
0.5162832622799883	0.3057576478348382	0.3706876570117603	T	T	T
0.8124234956531325	0.2912404348952601	0.3768331008680461	T	T	T
0.1538020478482730	0.2891574450662843	0.3766807678925821	T	T	T
0.4131595452019193	0.1208683607163741	0.4187857482324107	T	T	T
0.2777910000000006	0.8194148176612188	0.0136009167645312	F	F	F
0.2777910000000006	0.0396805729748735	0.0303792217909731	F	F	F
0.7222089999999994	0.8194148176612188	0.0136009167645312	F	F	F
0.7222089999999994	0.0396805729748735	0.0303792217909731	F	F	F
0.2222089999999994	0.7330449924233309	0.1065287437974050	F	F	F
0.2222089999999994	0.9533107477369782	0.1233070488238468	F	F	F
0.7777910000000006	0.7330449924233309	0.1065287437974050	F	F	F
0.7777910000000006	0.9533107477369782	0.1233070488238468	F	F	F
0.2930180107950127	0.5938399785726665	0.2811096435754751	T	T	T
0.3005086092793582	0.8238350445903339	0.2897858801635381	T	T	T
0.7014433343300203	0.6028576799599867	0.2799615494714289	T	T	T
0.7065724737968712	0.8355225515001744	0.2896260197503225	T	T	T
0.1889664882686899	0.7047268363163116	0.3546217005685712	T	T	T
0.1776519110921385	0.5265860549990687	0.3904150901992294	T	T	T
0.8458941715673689	0.6931412809314347	0.3473366833700473	T	T	T
0.9718606352353046	0.6816070187102902	0.3936410879316323	T	T	T
0.6935625213977070	0.2838271755204675	0.3809147055100880	T	T	T
0.0576913819317059	0.2313671040587226	0.3893054777706774	T	T	T
0.8402207971900211	0.4368118415736696	0.3792245411105023	T	T	T
0.3584551341267873	0.0627876624997278	0.3694869454629154	T	T	T
0.3243079064598952	0.2090081279814185	0.4209480831238791	T	T	T

Figure 2a State 4'

1.0000000000000000		
8.7372206091223994	0.0000000000000000	0.0000000000000000
0.0000000000000000	6.9809029500783426	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000

K	Ni	O	H
4	12	36	21

Selective dynamics

Direct

0.0000000000000000	0.9295476953180497	0.0219900692777486	F	F	F
0.5000000000000000	0.8431778700801544	0.1149178963106294	F	F	F
0.9996259326122331	0.7665676783601035	0.2104318666856763	T	T	T
0.5481734971150355	0.7404182756936040	0.3923406347870544	T	T	T
0.0000000000000000	0.4295476953180497	0.0219900692777486	F	F	F
0.3336660000000009	0.4295476953180497	0.0219900692777486	F	F	F
0.6663339999999991	0.4295476953180497	0.0219900692777486	F	F	F
0.1663339999999991	0.3431778700801544	0.1149178963106294	F	F	F
0.5000000000000000	0.3431778700801544	0.1149178963106294	F	F	F
0.8336660000000009	0.3431778700801544	0.1149178963106294	F	F	F
0.9993811259358634	0.2660885989634696	0.2098493112312496	T	T	T
0.3323871834154403	0.2607645739853565	0.2097238762956951	T	T	T
0.6666241452653848	0.2611619017828972	0.2092054823208307	T	T	T
0.1624999543930805	0.1915397190188799	0.3061788453385894	T	T	T
0.5047382665721034	0.1915760830653505	0.3049842636476940	T	T	T
0.8332490365305343	0.1918946773394664	0.3054826210806556	T	T	T

0.1735150000000019	0.5955569454815901	0.0004884286588833	F	F	F
0.5000000000000000	0.5859389052830437	0.0000000000000000	F	F	F
0.8264849999999981	0.5955569454815901	0.0004884286588833	F	F	F
0.1735150000000019	0.2635384451545022	0.0434917098966210	F	F	F
0.5000000000000000	0.2731564853530557	0.0439801385555043	F	F	F
0.8264849999999981	0.2635384451545022	0.0434917098966210	F	F	F
0.0000000000000000	0.4995690800451484	0.0929278270328737	F	F	F
0.3264849999999981	0.5091871202437019	0.0934162556917641	F	F	F
0.6735150000000019	0.5091871202437019	0.0934162556917641	F	F	F
0.0000000000000000	0.1867866601151604	0.1369079655883780	F	F	F
0.3264849999999981	0.1771686199166140	0.1364195369294947	F	F	F
0.6735150000000019	0.1771686199166140	0.1364195369294947	F	F	F
0.1667068184597698	0.4212667664734478	0.1870345633861255	T	T	T
0.4991120509354736	0.4166555544845597	0.1866047562771576	T	T	T
0.8327595944602905	0.4209067410590346	0.1871766215146518	T	T	T
0.1641739948142804	0.1100464652087278	0.2335774032455682	T	T	T
0.4997926542206435	0.1036201618953357	0.2318225792252222	T	T	T
0.8346373098455684	0.1095366726003066	0.2339487210378702	T	T	T
0.9973795349167123	0.3491873809144085	0.2817807534062928	T	T	T
0.3349960116723277	0.3451333985940133	0.2813925800638638	T	T	T
0.6626053458576513	0.3492278632034883	0.2807006554576058	T	T	T
0.9981680634150965	0.0388873200809391	0.3231802366538161	T	T	T
0.3446499707912140	0.0212670142007877	0.3252148801872323	T	T	T
0.6658078665852603	0.0335229790792356	0.3237493520104860	T	T	T
0.3436370000000011	0.9295476953180497	0.0219900692777486	F	F	F
0.6563629999999989	0.9295476953180497	0.0219900692777486	F	F	F
0.1563629999999989	0.8431778700801544	0.1149178963106294	F	F	F
0.8436370000000011	0.8431778700801544	0.1149178963106294	F	F	F
0.2222620945329868	0.6994044643148889	0.2857198641911188	T	T	T
0.7680351798741525	0.7137402083383007	0.2855703813703440	T	T	T
0.1826552408264015	0.6746819231546883	0.3935471117050567	T	T	T
0.8647676805476806	0.6557219178116805	0.3847553571224909	T	T	T
0.5124982284166272	0.3138920853357367	0.3739811117291911	T	T	T
0.8230961229823666	0.2928729555983763	0.3783257345870372	T	T	T
0.1664254178546335	0.2827874943138359	0.3783723691624886	T	T	T
0.4317344995807410	0.2134809564117629	0.4151460789342883	T	T	T
0.2777910000000006	0.8194148176612188	0.0136009167645312	F	F	F
0.2777910000000006	0.0396805729748735	0.0303792217909731	F	F	F
0.7222089999999994	0.8194148176612188	0.0136009167645312	F	F	F
0.7222089999999994	0.0396805729748735	0.0303792217909731	F	F	F
0.2222089999999994	0.7330449924233307	0.1065287437974050	F	F	F
0.2222089999999994	0.9533107477369782	0.1233070488238468	F	F	F
0.7777910000000006	0.7330449924233307	0.1065287437974050	F	F	F
0.7777910000000006	0.9533107477369782	0.1233070488238468	F	F	F
0.2820885759817889	0.5792625678716351	0.2811742365544687	T	T	T
0.2929904131148477	0.8083616180268718	0.2888395321741793	T	T	T
0.7014077443896540	0.6029021345179816	0.2780569718873900	T	T	T
0.7080803768166010	0.8357638952995364	0.2898816262208329	T	T	T
0.1868059521234178	0.6988061073695346	0.3539786289942150	T	T	T
0.1780590699678266	0.5320788035794399	0.3936239067695298	T	T	T
0.8486696621384693	0.6910080855766830	0.3459211662410711	T	T	T
0.9741621252429967	0.6867737982214511	0.3928220133384431	T	T	T
0.7099157327980022	0.2814686430518992	0.3847396105520144	T	T	T
0.0752424561540142	0.2204821857926762	0.3933972395912717	T	T	T
0.8474244410207973	0.4395516578612234	0.3802462851215018	T	T	T
0.3400974545404660	0.0322900431738088	0.3645036915714031	T	T	T
0.3176072083335286	0.2495207075219358	0.4059548158113502	T	T	T

Figure 2a State 5

1.0000000000000000

8.7372206091223994      0.0000000000000000      0.0000000000000000

0.0000000000000000	6.9809029500783426	0.0000000000000000			
0.0000000000000000	0.0000000000000000	25.0000000000000000			
K	Ni	O	H		
4	12	36	20		
Selective dynamics					
Direct					
0.0000000000000000	0.9295476953180497	0.0219900692777486	F	F	F
0.5000000000000000	0.8431778700801544	0.1149178963106294	F	F	F
0.9983452928211569	0.7646414881080978	0.2111192856125320	T	T	T
0.5232303530657167	0.7581573107448636	0.3921845721800574	T	T	T
0.0000000000000000	0.4295476953180497	0.0219900692777486	F	F	F
0.3336660000000009	0.4295476953180497	0.0219900692777486	F	F	F
0.6663339999999991	0.4295476953180497	0.0219900692777486	F	F	F
0.1663339999999991	0.3431778700801544	0.1149178963106294	F	F	F
0.5000000000000000	0.3431778700801544	0.1149178963106294	F	F	F
0.8336660000000009	0.3431778700801544	0.1149178963106294	F	F	F
0.0004123192454195	0.2634766112300979	0.2096038800479971	T	T	T
0.3335138524070798	0.2596233252109716	0.2096241240061625	T	T	T
0.6669679062630043	0.2598999984396291	0.2093688091355524	T	T	T
0.1624885321404662	0.1848823907970872	0.3049342451340939	T	T	T
0.5050603484602635	0.1940622854411244	0.3060547692254907	T	T	T
0.8355809668022401	0.1873262350368465	0.3054427125357251	T	T	T
0.1735150000000019	0.5955569454815901	0.0004884286588833	F	F	F
0.5000000000000000	0.5859389052830437	0.0000000000000000	F	F	F
0.8264849999999981	0.5955569454815901	0.0004884286588833	F	F	F
0.1735150000000019	0.2635384451545022	0.0434917098966210	F	F	F
0.5000000000000000	0.2731564853530557	0.0439801385555043	F	F	F
0.8264849999999981	0.2635384451545022	0.0434917098966210	F	F	F
0.0000000000000000	0.4995690800451484	0.0929278270328737	F	F	F
0.3264849999999981	0.5091871202437019	0.0934162556917641	F	F	F
0.6735150000000019	0.5091871202437019	0.0934162556917641	F	F	F
0.0000000000000000	0.1867866601151604	0.1369079655883780	F	F	F
0.3264849999999981	0.1771686199166140	0.1364195369294947	F	F	F
0.6735150000000019	0.1771686199166140	0.1364195369294947	F	F	F
0.1677974979271052	0.4206333060699231	0.1871435413098791	T	T	T
0.4997682939840803	0.4161993395396454	0.1867702231660584	T	T	T
0.8333513539709997	0.4191496204031795	0.1874837416353490	T	T	T
0.1664376678987627	0.1065257484809525	0.2324567073436220	T	T	T
0.5001806035652466	0.1018199029655497	0.2322499422984310	T	T	T
0.8333513438976872	0.1073149757420024	0.2338981069199498	T	T	T
0.0007201763774439	0.3430092942896162	0.2817652629443747	T	T	T
0.3352803584289662	0.3438793372002562	0.2813217347978627	T	T	T
0.6653755766225228	0.3484502626157557	0.2807458853858891	T	T	T
0.9988418326132665	0.0272716313378055	0.3201061831427107	T	T	T
0.3437762792283018	0.0289281577632407	0.3307668214578002	T	T	T
0.6661106411993802	0.0371018837703574	0.3260815039745765	T	T	T
0.3436370000000011	0.9295476953180497	0.0219900692777486	F	F	F
0.6563629999999989	0.9295476953180497	0.0219900692777486	F	F	F
0.1563629999999989	0.8431778700801544	0.1149178963106294	F	F	F
0.8436370000000011	0.8431778700801544	0.1149178963106294	F	F	F
0.2278820242825651	0.7001439574077741	0.2852886685770167	T	T	T
0.7705835532105166	0.7099177244394047	0.2909020303406278	T	T	T
0.1871607661106059	0.6490394245391151	0.3928897285157552	T	T	T
0.8672517743277584	0.6390284233071335	0.3884017625051332	T	T	T
0.5067724181157377	0.3310264698231041	0.3728819545755424	T	T	T
0.8477187506425669	0.2836573345215075	0.3793025603406646	T	T	T
0.1696899079678804	0.2616604593870648	0.3768502869417029	T	T	T
0.5316222850029027	0.2355600772778731	0.4165503568846112	T	T	T
0.2777910000000006	0.8194148176612188	0.0136009167645312	F	F	F
0.2777910000000006	0.0396805729748735	0.0303792217909731	F	F	F
0.7222089999999994	0.8194148176612188	0.0136009167645312	F	F	F

0.7222089999999994	0.0396805729748735	0.0303792217909731	F	F	F
0.2222089999999994	0.7330449924233307	0.1065287437974050	F	F	F
0.2222089999999994	0.9533107477369782	0.1233070488238468	F	F	F
0.7777910000000006	0.7330449924233307	0.1065287437974050	F	F	F
0.7777910000000006	0.9533107477369782	0.1233070488238468	F	F	F
0.2869973101959853	0.5799580911364787	0.2797012043029651	T	T	T
0.2981231485586447	0.8090672910769667	0.2870929825280672	T	T	T
0.7052788309983931	0.5989715358117114	0.2817426168564987	T	T	T
0.7108736584435693	0.8323037440847600	0.2939229521705475	T	T	T
0.1903843402285280	0.6837665856784789	0.3540414868671658	T	T	T
0.1870745906273877	0.5055232025037290	0.3907234883506905	T	T	T
0.8464180413781658	0.6793477761037290	0.3499751936094523	T	T	T
0.9787519413527559	0.6649567955829718	0.3948776839180932	T	T	T
0.7568057627391084	0.2317090879158731	0.3971785901364142	T	T	T
0.0681060866496722	0.2212879123406008	0.3896813001879742	T	T	T
0.8525144528574492	0.4374848412681684	0.3837554473321518	T	T	T
0.3095432137522667	0.0809271313854266	0.3662695129565170	T	T	T

Figure 3a State 1 (NUPDOWN=8)

1.000000000000000					
8.7372206091223994	0.0000000000000000	0.0000000000000000			
0.0000000000000000	6.9809029500783426	0.0000000000000000			
0.0000000000000000	0.0000000000000000	25.0000000000000000			
K	Ni	O	H	Fe	
4	11	34	20	1	
Selective dynamics					
Direct					
0.0000000000000000	0.9295476953180497	0.0219900692777486	F	F	F
0.5000000000000000	0.8431778700801544	0.1149178963106294	F	F	F
0.9886082611786221	0.7603904672520053	0.2114914777555677	T	T	T
0.6132325239553661	0.6810356961587424	0.3472494051452178	T	T	T
0.0000000000000000	0.4295476953180497	0.0219900692777486	F	F	F
0.3336660000000009	0.4295476953180497	0.0219900692777486	F	F	F
0.6663339999999991	0.4295476953180497	0.0219900692777486	F	F	F
0.1663339999999991	0.3431778700801544	0.1149178963106294	F	F	F
0.5000000000000000	0.3431778700801544	0.1149178963106294	F	F	F
0.8336660000000009	0.3431778700801544	0.1149178963106294	F	F	F
0.9984611754259736	0.2622377059756983	0.2103730046850541	T	T	T
0.3328424228632799	0.2534836906059333	0.2100180390197892	T	T	T
0.6662442500286512	0.2577841241916031	0.2095729035335220	T	T	T
0.1655509059268202	0.1751190804970507	0.3062604759010414	T	T	T
0.5120511082419039	0.1742886419122253	0.3066092158055218	T	T	T
0.1735150000000019	0.5955569454815901	0.0004884286588833	F	F	F
0.5000000000000000	0.5859389052830437	0.0000000000000000	F	F	F
0.8264849999999981	0.5955569454815901	0.0004884286588833	F	F	F
0.1735150000000019	0.2635384451545022	0.0434917098966210	F	F	F
0.5000000000000000	0.2731564853530557	0.0439801385555043	F	F	F
0.8264849999999981	0.2635384451545022	0.0434917098966210	F	F	F
0.0000000000000000	0.4995690800451484	0.0929278270328737	F	F	F
0.3264849999999981	0.5091871202437019	0.0934162556917641	F	F	F
0.6735150000000019	0.5091871202437019	0.0934162556917641	F	F	F
0.0000000000000000	0.1867866601151604	0.1369079655883780	F	F	F
0.3264849999999981	0.1771686199166140	0.1364195369294947	F	F	F
0.6735150000000019	0.1771686199166140	0.1364195369294947	F	F	F
0.1673804482501297	0.4164714681372306	0.1882588076270456	T	T	T
0.4983052984871877	0.4141645721187200	0.1876164274944625	T	T	T
0.8319309976592976	0.4184180948639436	0.1873945367868982	T	T	T
0.1641383560404966	0.1010841946108347	0.2338979090266442	T	T	T
0.5006955226103921	0.0919116475627060	0.2254506473500670	T	T	T
0.8315374882705662	0.1054260637370339	0.2341947062473919	T	T	T
0.9900093030419032	0.3558581453741846	0.2795270118788328	T	T	T

0.3396178356870813	0.3229527200502171	0.2839897103093511	T	T	T
0.6611796444217838	0.3411392270618830	0.2814116651559390	T	T	T
0.9903231849908061	0.0274781776934544	0.3220476831427614	T	T	T
0.3628593433524835	-0.0020515274355561	0.3314828643601295	T	T	T
0.6774086919450876	0.0579797897835563	0.3351104739155926	T	T	T
0.3436370000000011	0.9295476953180497	0.0219900692777486	F	F	F
0.6563629999999989	0.9295476953180497	0.0219900692777486	F	F	F
0.1563629999999989	0.8431778700801544	0.1149178963106294	F	F	F
0.8436370000000011	0.8431778700801544	0.1149178963106294	F	F	F
0.2195102522394222	0.6860236200509909	0.2923841884328131	T	T	T
0.6106905862804558	0.7364805927898649	0.2418648426488815	T	T	T
0.2307878982567967	0.6186300127180170	0.3972746101795390	T	T	T
0.9115409165689816	0.7238894781920980	0.3945363362799960	T	T	T
0.8561660620769235	0.3330282186345280	0.3732340806269061	T	T	T
0.1574638508500490	0.2591253814477457	0.3812620832186624	T	T	T
0.2777910000000006	0.8194148176612188	0.0136009167645312	F	F	F
0.2777910000000006	0.0396805729748735	0.0303792217909731	F	F	F
0.7222089999999994	0.8194148176612188	0.0136009167645312	F	F	F
0.7222089999999994	0.0396805729748735	0.0303792217909731	F	F	F
0.2222089999999994	0.7330449924233307	0.1065287437974050	F	F	F
0.2222089999999994	0.9533107477369782	0.1233070488238468	F	F	F
0.7777910000000006	0.7330449924233307	0.1065287437974050	F	F	F
0.7777910000000006	0.9533107477369782	0.1233070488238468	F	F	F
0.2774598254260269	0.5693827353899413	0.2823034671293724	T	T	T
0.2905220430583856	0.7958018743370743	0.2959946284053268	T	T	T
0.5596469848178759	0.6314558096693677	0.2224104963742602	T	T	T
0.5589469119512566	0.8589486114159600	0.2330507496656536	T	T	T
0.2192221156446860	0.6526630028214234	0.3581265139904660	T	T	T
0.1345183107097004	0.6678278932707629	0.4127420908500836	T	T	T
0.9089510899700172	0.5927733385113373	0.3796116859143433	T	T	T
0.9440765046103705	0.8137412314662851	0.3661007517452904	T	T	T
0.3466897367130128	0.0058060052237458	0.3701228202106294	T	T	T
0.7892538153467832	0.2681577809745261	0.3987781659210664	T	T	T
0.0428013475159137	0.2728402476018456	0.3857175380130268	T	T	T
0.1971034642359444	0.3955348607517054	0.3880241136320158	T	T	T
0.8393150788526442	0.1901016653913669	0.3079652407174324	T	T	T

Figure 3a State 2 (NUPDOWN=7)

1.0000000000000000		
8.7372206091223994	0.0000000000000000	0.0000000000000000
0.0000000000000000	6.9809029500783426	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000

K	Ni	O	H	Fe
4	11	35	21	1

Selective dynamics

Direct

0.0000000000000000	0.9295476953180497	0.0219900692777486	F	F	F
0.5000000000000000	0.8431778700801544	0.1149178963106294	F	F	F
0.0417236811696230	0.7600503051721114	0.2080112341784389	T	T	T
0.5229306827101077	0.7111068325470234	0.3470182838460086	T	T	T
0.0000000000000000	0.4295476953180497	0.0219900692777486	F	F	F
0.3336660000000009	0.4295476953180497	0.0219900692777486	F	F	F
0.6663339999999991	0.4295476953180497	0.0219900692777486	F	F	F
0.1663339999999991	0.3431778700801544	0.1149178963106294	F	F	F
0.5000000000000000	0.3431778700801544	0.1149178963106294	F	F	F
0.8336660000000009	0.3431778700801544	0.1149178963106294	F	F	F
0.0001617414885252	0.2589431821732199	0.2106570095865224	T	T	T
0.3332869982253721	0.2553516237610066	0.2099442286872139	T	T	T
0.6660733019932268	0.2562339237271297	0.2100902218286555	T	T	T
0.1690090624058210	0.1831850311794231	0.3071452430021370	T	T	T
0.5022756103714781	0.1877215219505889	0.3074830416350440	T	T	T



0.1735150000000019	0.5955569454815901	0.0004884286588833	F	F	F
0.5000000000000000	0.5859389052830437	0.0000000000000000	F	F	F
0.8264849999999981	0.5955569454815901	0.0004884286588833	F	F	F
0.1735150000000019	0.2635384451545022	0.0434917098966210	F	F	F
0.5000000000000000	0.2731564853530557	0.0439801385555043	F	F	F
0.8264849999999981	0.2635384451545022	0.0434917098966210	F	F	F
0.0000000000000000	0.4995690800451484	0.0929278270328737	F	F	F
0.3264849999999981	0.5091871202437019	0.0934162556917641	F	F	F
0.6735150000000019	0.5091871202437019	0.0934162556917641	F	F	F
0.0000000000000000	0.1867866601151604	0.1369079655883780	F	F	F
0.3264849999999981	0.1771686199166140	0.1364195369294947	F	F	F
0.6735150000000019	0.1771686199166140	0.1364195369294947	F	F	F
0.1660186943794546	0.4146099630309170	0.1880282792865484	T	T	T
0.4993590945360228	0.4148390107590116	0.1878280570635924	T	T	T
0.8319832008300971	0.4193039283956296	0.1882900478697744	T	T	T
0.1672127370094466	0.1017618874407111	0.2341693650650938	T	T	T
0.4986902655511025	0.0943114886033333	0.2284498532084103	T	T	T
0.8317383442150829	0.1006420632048877	0.2341921767350766	T	T	T
0.0011801474917227	0.3431750631530620	0.2817543553729223	T	T	T
0.3362705288827249	0.3376420380742191	0.2817417065578295	T	T	T
0.6651567372494274	0.3417791558277153	0.2813724977180363	T	T	T
0.9924104409616984	0.0325264504254888	0.3250767653223136	T	T	T
0.3413233288733305	0.0388245229390890	0.3286793231440426	T	T	T
0.6741815961490397	0.0408649867764547	0.3288791355484667	T	T	T
0.3436370000000011	0.9295476953180497	0.0219900692777486	F	F	F
0.6563629999999989	0.9295476953180497	0.0219900692777486	F	F	F
0.1563629999999989	0.8431778700801544	0.1149178963106294	F	F	F
0.8436370000000011	0.8431778700801544	0.1149178963106294	F	F	F
0.3533294549155023	0.7275703041496652	0.2460524787801949	T	T	T
0.7331432770660490	0.7281137384684665	0.2545429194508331	T	T	T
0.2020754864152016	0.6434174847723622	0.3486043968589283	T	T	T
0.8820421389867180	0.6936099114168911	0.3496403847868138	T	T	T
0.5341942664156880	0.3435487656197248	0.3884569708929577	T	T	T
0.8376738386641004	0.3165926539323956	0.3756784198092318	T	T	T
0.1568825279776663	0.2945470523110798	0.3789383528055137	T	T	T
0.2777910000000006	0.8194148176612188	0.0136009167645312	F	F	F
0.2777910000000006	0.0396805729748735	0.0303792217909731	F	F	F
0.7222089999999994	0.8194148176612188	0.0136009167645312	F	F	F
0.7222089999999994	0.0396805729748735	0.0303792217909731	F	F	F
0.2222089999999994	0.7330449924233307	0.1065287437974050	F	F	F
0.2222089999999994	0.9533107477369782	0.1233070488238468	F	F	F
0.7777910000000006	0.7330449924233307	0.1065287437974050	F	F	F
0.7777910000000006	0.9533107477369782	0.1233070488238468	F	F	F
0.4180894244779174	0.6307914301482729	0.2284460601071218	T	T	T
0.4056897929820037	0.8523944841305120	0.2431818612518224	T	T	T
0.7506581073222025	0.6303182205100870	0.2267383893116992	T	T	T
0.7525220431393138	0.8575245899817874	0.2399492760908575	T	T	T
0.2395601121025830	0.6493983602318552	0.3113258748902262	T	T	T
0.0922917268009867	0.6791088997597493	0.3466898086131764	T	T	T
0.8375762861656942	0.6960270156833576	0.3127485239560484	T	T	T
0.9065923684043340	0.8305412589374351	0.3558849241005375	T	T	T
0.6476936209144147	0.3156015593780530	0.3915448484600433	T	T	T
0.4782843232257073	0.2602896798189018	0.4128799974162382	T	T	T
0.0437784707564752	0.2893740286589170	0.3862934479797454	T	T	T
0.8550924422858046	0.4545720062997951	0.3678302046968385	T	T	T
0.1799542136983914	0.4357016761279258	0.3694439434622796	T	T	T
0.8346525014712527	0.1832924535468215	0.3094242328237768	T	T	T

Figure 3a State 3 (NUPDOWN=8)

1.0000000000000000

8.7372206091223994      0.0000000000000000      0.0000000000000000



0.0000000000000000	6.9809029500783426	0.0000000000000000			
0.0000000000000000	0.0000000000000000	25.0000000000000000			
K	Ni	O	H	Fe	
4	11	36	22	1	
Selective dynamics					
Direct					
0.0000000000000000	0.9295476953180497	0.0219900692777486	F	F	F
0.5000000000000000	0.8431778700801544	0.1149178963106294	F	F	F
0.9839951121149492	0.7652201587931456	0.2115048044098938	T	T	T
0.5479514828494358	0.7301788016718088	0.3927563324282417	T	T	T
0.0000000000000000	0.4295476953180497	0.0219900692777486	F	F	F
0.3336660000000009	0.4295476953180497	0.0219900692777486	F	F	F
0.6663339999999991	0.4295476953180497	0.0219900692777486	F	F	F
0.1663339999999991	0.3431778700801544	0.1149178963106294	F	F	F
0.5000000000000000	0.3431778700801544	0.1149178963106294	F	F	F
0.8336660000000009	0.3431778700801544	0.1149178963106294	F	F	F
0.9984412633916662	0.2627299651670623	0.2102874779023590	T	T	T
0.3321454101711785	0.2662708308865315	0.2101408080387257	T	T	T
0.6673364145774336	0.2620217596859303	0.2095711587454400	T	T	T
0.1574518405772844	0.1938759932179863	0.3069718455332091	T	T	T
0.5031412609390128	0.2081525349090604	0.3053795358860961	T	T	T
0.1735150000000019	0.5955569454815901	0.0004884286588833	F	F	F
0.5000000000000000	0.5859389052830437	0.0000000000000000	F	F	F
0.8264849999999981	0.5955569454815901	0.0004884286588833	F	F	F
0.1735150000000019	0.2635384451545022	0.0434917098966210	F	F	F
0.5000000000000000	0.2731564853530557	0.0439801385555043	F	F	F
0.8264849999999981	0.2635384451545022	0.0434917098966210	F	F	F
0.0000000000000000	0.4995690800451484	0.0929278270328737	F	F	F
0.3264849999999981	0.5091871202437019	0.0934162556917641	F	F	F
0.6735150000000019	0.5091871202437019	0.0934162556917641	F	F	F
0.0000000000000000	0.1867866601151604	0.1369079655883780	F	F	F
0.3264849999999981	0.1771686199166140	0.1364195369294947	F	F	F
0.6735150000000019	0.1771686199166140	0.1364195369294947	F	F	F
0.1653283250528341	0.4214633237004026	0.1869997548245611	T	T	T
0.4990852249154765	0.4179816432606312	0.1865940597448888	T	T	T
0.8339397102738060	0.4179713389250756	0.1869350540128065	T	T	T
0.1674256720513178	0.1125900379167252	0.2350866823539585	T	T	T
0.4973906875131307	0.1118185940684947	0.2340034573726350	T	T	T
0.8315540135433693	0.1081201955327019	0.2320173402019496	T	T	T
0.9946647205364065	0.3409176799069267	0.2819567334792479	T	T	T
0.3396266617782817	0.3634645639056523	0.2795744739119859	T	T	T
0.6654288422345971	0.3542377568584756	0.2793102273146362	T	T	T
0.9651234008274261	0.0029327598690633	0.3227548209001407	T	T	T
0.3345049818487194	0.0452850519920279	0.3269231369467894	T	T	T
0.6582569740233454	0.0357634807229846	0.3225027185579147	T	T	T
0.3436370000000011	0.9295476953180497	0.0219900692777486	F	F	F
0.6563629999999989	0.9295476953180497	0.0219900692777486	F	F	F
0.1563629999999989	0.8431778700801544	0.1149178963106294	F	F	F
0.8436370000000011	0.8431778700801544	0.1149178963106294	F	F	F
0.2194955062527602	0.7083942119721661	0.2911054661954145	T	T	T
0.6465217555466346	0.7595956335659180	0.2177513594414839	T	T	T
0.1909191114551553	0.6367488213922859	0.3951132435039009	T	T	T
0.8684490535609805	0.7024363128185689	0.3894492864718456	T	T	T
0.5197448178180675	0.3263563900089112	0.3731073264282830	T	T	T
0.8349306913727508	0.3090015977864162	0.3692811200835420	T	T	T
0.1295941461872936	0.2759951526054287	0.3805545742838359	T	T	T
0.4057059216248230	0.0542061136331458	0.4322133198441627	T	T	T
0.2777910000000006	0.8194148176612188	0.0136009167645312	F	F	F
0.2777910000000006	0.0396805729748735	0.0303792217909731	F	F	F
0.7222089999999994	0.8194148176612188	0.0136009167645312	F	F	F
0.7222089999999994	0.0396805729748735	0.0303792217909731	F	F	F

0.2222089999999994	0.7330449924233307	0.1065287437974050	F	F	F
0.2222089999999994	0.9533107477369782	0.1233070488238468	F	F	F
0.7777910000000006	0.7330449924233307	0.1065287437974050	F	F	F
0.7777910000000006	0.9533107477369782	0.1233070488238468	F	F	F
0.2839862894013123	0.5955188135567890	0.2817176016875710	T	T	T
0.2833043249980200	0.8247210943191594	0.2934032300036657	T	T	T
0.5941657360654676	0.6394781193883934	0.2262666574510808	T	T	T
0.6150433732122206	0.8541701719045661	0.2444835696427286	T	T	T
0.1948892448356880	0.6720817914443158	0.3558255188130284	T	T	T
0.0868588140456039	0.6780845284468086	0.4057877195952734	T	T	T
0.8641988211831007	0.5743404442497951	0.3722390880753601	T	T	T
0.8964724912183812	0.7983839619053846	0.3617277379496074	T	T	T
0.4534814363817729	0.1746531553497738	0.4158280366491081	T	T	T
0.0113594516562476	0.2823282823566658	0.3826038352871274	T	T	T
0.1635726552612804	0.4162911946498308	0.3865704296092742	T	T	T
0.6335128581994791	0.3186153073561222	0.3782102232119543	T	T	T
0.3129272821167189	0.0958321772338939	0.4503982955875147	T	T	T
0.3376609206411639	0.0405565030588820	0.3672005516921348	T	T	T
0.8287473689183962	0.1768856911207929	0.3104818811028817	T	T	T

Figure 3a State 3 → 3-Ni' TS (NUPDOWN=8)

1.000000000000000		
8.7372206091223994	0.0000000000000000	0.0000000000000000
0.0000000000000000	6.9809029500783426	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000

K Ni O H Fe

4 11 36 22 1

Selective dynamics

Direct

0.0000000000000000	0.9295476953180499	0.0219900692777486	F	F	F
0.5000000000000000	0.8431778700801544	0.1149178963106294	F	F	F
0.9857184325676328	0.7593151522703165	0.2113469227922584	T	T	T
0.5802253670659588	0.6744788448520370	0.3516745040069886	T	T	T
0.0000000000000000	0.4295476953180497	0.0219900692777486	F	F	F
0.3336660000000009	0.4295476953180497	0.0219900692777486	F	F	F
0.6663339999999991	0.4295476953180497	0.0219900692777486	F	F	F
0.1663339999999991	0.3431778700801547	0.1149178963106294	F	F	F
0.5000000000000000	0.3431778700801547	0.1149178963106294	F	F	F
0.8336660000000009	0.3431778700801547	0.1149178963106294	F	F	F
0.9985368560046421	0.2610572308681704	0.2101497247383394	T	T	T
0.3319392817084768	0.2558378522054053	0.2096252787640039	T	T	T
0.6675693893359220	0.2574295213669098	0.2096312044921581	T	T	T
0.1603729970034682	0.1755990649079694	0.3080723838594054	T	T	T
0.5064294415903664	0.1798151726029335	0.3051653639782578	T	T	T
0.1735150000000019	0.5955569454815901	0.0004884286588833	F	F	F
0.5000000000000000	0.5859389052830437	0.0000000000000000	F	F	F
0.8264849999999981	0.5955569454815901	0.0004884286588833	F	F	F
0.1735150000000019	0.2635384451545022	0.0434917098966210	F	F	F
0.5000000000000000	0.2731564853530558	0.0439801385555043	F	F	F
0.8264849999999981	0.2635384451545022	0.0434917098966210	F	F	F
0.0000000000000000	0.4995690800451488	0.0929278270328737	F	F	F
0.3264849999999981	0.5091871202437019	0.0934162556917641	F	F	F
0.6735150000000019	0.5091871202437019	0.0934162556917641	F	F	F
0.0000000000000000	0.1867866601151605	0.1369079655883780	F	F	F
0.3264849999999981	0.1771686199166141	0.1364195369294947	F	F	F
0.6735150000000019	0.1771686199166141	0.1364195369294947	F	F	F
0.1663201903529074	0.4178092859447632	0.1879206570220215	T	T	T
0.5005715939997446	0.4146731783203152	0.1874594483679725	T	T	T
0.8320614731267759	0.4182195316489594	0.1874028254390192	T	T	T
0.1635593298090088	0.1035337473966467	0.2316469242543860	T	T	T
0.5007252136740463	0.0958703303472230	0.2291835630179737	T	T	T

0.8333283024019271	0.1019512770638805	0.2325325836984635	T	T	T
0.9867841607545592	0.3429886782244270	0.2813940680432989	T	T	T
0.3377009223946744	0.3325371406429469	0.2816284186051635	T	T	T
0.6657665156518592	0.3396690027732658	0.2814466227798603	T	T	T
0.9819366140121278	0.0111026871404271	0.3248802923675105	T	T	T
0.3492778452084775	0.0053588308261171	0.3276226658002822	T	T	T
0.6739098564195510	0.0281412962451522	0.3245023909859783	T	T	T
0.3436370000000011	0.9295476953180499	0.0219900692777486	F	F	F
0.6563629999999989	0.9295476953180499	0.0219900692777486	F	F	F
0.1563629999999989	0.8431778700801544	0.1149178963106294	F	F	F
0.8436370000000011	0.8431778700801544	0.1149178963106294	F	F	F
0.2153222224169831	0.6914462130248504	0.2881181551446621	T	T	T
0.6134684198151129	0.7314902174088534	0.2435425188404094	T	T	T
0.2142805683754581	0.6518181619712268	0.3939094641271488	T	T	T
0.8839480158666472	0.7173001675738195	0.3933684158652196	T	T	T
0.5016911639857378	0.2840745166505538	0.3778284175157852	T	T	T
0.8341702165457922	0.2955591185066078	0.3775076225270271	T	T	T
0.1491364274028426	0.2896798262991102	0.3853408137904635	T	T	T
0.4223557847900949	0.1450029838979053	0.4300221008460235	T	T	T
0.2777910000000006	0.8194148176612188	0.0136009167645312	F	F	F
0.2777910000000006	0.0396805729748735	0.0303792217909731	F	F	F
0.7222089999999994	0.8194148176612188	0.0136009167645312	F	F	F
0.7222089999999994	0.0396805729748735	0.0303792217909731	F	F	F
0.2222089999999994	0.7330449924233309	0.1065287437974050	F	F	F
0.2222089999999994	0.9533107477369782	0.1233070488238468	F	F	F
0.7777910000000006	0.7330449924233309	0.1065287437974050	F	F	F
0.7777910000000006	0.9533107477369782	0.1233070488238468	F	F	F
0.2757936531959587	0.5742761081100474	0.2801746065861641	T	T	T
0.2849251226693374	0.8027637334085151	0.2918750835224895	T	T	T
0.5620917130474087	0.6295953679186427	0.2229606880388270	T	T	T
0.5633432768909955	0.8551326068373328	0.2356070721002655	T	T	T
0.2023170129296626	0.6779337011744903	0.3543228567639140	T	T	T
0.1198176452417023	0.7029843181269660	0.4098479209066638	T	T	T
0.8922098431936737	0.5848558115198104	0.3805435171649607	T	T	T
0.9187513707216106	0.8035860116862833	0.3642127540210367	T	T	T
0.3575556719560725	0.0094049896759454	0.3672757018287491	T	T	T
0.0349882927801391	0.2935127635886420	0.3887460827353399	T	T	T
0.1812223752275982	0.4311046959392578	0.3886749780748934	T	T	T
0.8303890228806805	0.1914448918932179	0.4037102916043249	T	T	T
0.3194204997394824	0.2041400613342232	0.4262444756274863	T	T	T
0.6102336060233456	0.2679495937276845	0.3891936306919201	T	T	T
0.8351610411242538	0.1703115281811189	0.3073517278432724	T	T	T

Figure 3a State 3-Ni' (NUPDOWN=8)

1.0000000000000000		
8.7372206091223994	0.0000000000000000	0.0000000000000000
0.0000000000000000	6.9809029500783426	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000

K	Ni	O	H	Fe
4	11	36	22	1

Selective dynamics

Direct

0.0000000000000000	0.9295476953180497	0.0219900692777486	F	F	F
0.5000000000000000	0.8431778700801544	0.1149178963106294	F	F	F
0.9837933459620782	0.7643599611899964	0.2100523809011207	T	T	T
0.5862251568570768	0.6548184879226399	0.3423259100749018	T	T	T
0.0000000000000000	0.4295476953180497	0.0219900692777486	F	F	F
0.3336660000000009	0.4295476953180497	0.0219900692777486	F	F	F
0.6663339999999991	0.4295476953180497	0.0219900692777486	F	F	F
0.1663339999999991	0.3431778700801544	0.1149178963106294	F	F	F
0.5000000000000000	0.3431778700801544	0.1149178963106294	F	F	F

0.8336660000000009	0.3431778700801544	0.1149178963106294	F	F	F
0.0000554047860480	0.2659475762414141	0.2097267963842668	T	T	T
0.3323376970210305	0.2571753695612188	0.2103096194383237	T	T	T
0.6682624751533625	0.2593035326869752	0.2103868329326868	T	T	T
0.1643089850003440	0.1854705497579510	0.3075399489401382	T	T	T
0.5065610752591370	0.1801058120876043	0.3080447517769073	T	T	T
0.1735150000000019	0.5955569454815901	0.0004884286588833	F	F	F
0.5000000000000000	0.5859389052830437	0.0000000000000000	F	F	F
0.8264849999999981	0.5955569454815901	0.0004884286588833	F	F	F
0.1735150000000019	0.2635384451545022	0.0434917098966210	F	F	F
0.5000000000000000	0.2731564853530557	0.0439801385555043	F	F	F
0.8264849999999981	0.2635384451545022	0.0434917098966210	F	F	F
0.0000000000000000	0.4995690800451484	0.0929278270328737	F	F	F
0.3264849999999981	0.5091871202437019	0.0934162556917641	F	F	F
0.6735150000000019	0.5091871202437019	0.0934162556917641	F	F	F
0.0000000000000000	0.1867866601151604	0.1369079655883780	F	F	F
0.3264849999999981	0.1771686199166140	0.1364195369294947	F	F	F
0.6735150000000019	0.1771686199166140	0.1364195369294947	F	F	F
0.1684080485521098	0.4190967979428495	0.1873193550893595	T	T	T
0.4999727738400945	0.4140724814315502	0.1876842441539911	T	T	T
0.8308470948906022	0.4206956225733717	0.1866943553949065	T	T	T
0.1647863459609869	0.1066829695331973	0.2335448647020115	T	T	T
0.5021568615893857	0.1000560960768395	0.2336930983523897	T	T	T
0.8359452152869413	0.1090512774668532	0.2338263517208508	T	T	T
0.9907331905706347	0.3615774079131116	0.2790230866060854	T	T	T
0.3343470486176949	0.3339441659175122	0.2834533575366360	T	T	T
0.6664754636336708	0.3402192864599851	0.2828537830441676	T	T	T
0.9924324723300078	0.0335943195877826	0.3238399087242417	T	T	T
0.3496821020729774	0.0030603023746834	0.3268578421878859	T	T	T
0.6831456778458216	0.0227304988155570	0.3322323531523482	T	T	T
0.3436370000000011	0.9295476953180497	0.0219900692777486	F	F	F
0.6563629999999989	0.9295476953180497	0.0219900692777486	F	F	F
0.1563629999999989	0.8431778700801544	0.1149178963106294	F	F	F
0.8436370000000011	0.8431778700801544	0.1149178963106294	F	F	F
0.2138704573626031	0.6932404682667540	0.2867011303477559	T	T	T
0.6165744110397591	0.7383851735012380	0.2371691704329528	T	T	T
0.2018760031049507	0.6541075049201949	0.3923095350294798	T	T	T
0.8861183938438234	0.7258861309806836	0.3907527274862615	T	T	T
0.5110702885157196	0.2944838695758070	0.3771426356600212	T	T	T
0.8514939234167780	0.3361548324959674	0.3729454844899388	T	T	T
0.1563455965416927	0.2914124109648900	0.3843471031820407	T	T	T
0.4399511661590487	0.1854033665200593	0.4187242903458682	T	T	T
0.2777910000000006	0.8194148176612188	0.0136009167645312	F	F	F
0.2777910000000006	0.0396805729748735	0.0303792217909731	F	F	F
0.7222089999999994	0.8194148176612188	0.0136009167645312	F	F	F
0.7222089999999994	0.0396805729748735	0.0303792217909731	F	F	F
0.2222089999999994	0.7330449924233307	0.1065287437974050	F	F	F
0.2222089999999994	0.9533107477369782	0.1233070488238468	F	F	F
0.7777910000000006	0.7330449924233307	0.1065287437974050	F	F	F
0.7777910000000006	0.9533107477369782	0.1233070488238468	F	F	F
0.2728160721948774	0.5743024672179016	0.2795600046715945	T	T	T
0.2843424803134880	0.8037894616348338	0.2897007685499757	T	T	T
0.5614562689431278	0.6348628023939580	0.2183272961843281	T	T	T
0.5608680384815550	0.8608733022894002	0.2326829031486415	T	T	T
0.1969703774101504	0.6795528731217347	0.3524582400328110	T	T	T
0.1011217627555442	0.6999293904709407	0.4053017463605886	T	T	T
0.8858820720559999	0.5909023143807204	0.3777329109999940	T	T	T
0.9179276790396320	0.8108260275322743	0.3611505465033506	T	T	T
0.3503249714875012	0.9928588523415692	0.3660943050870733	T	T	T
0.0433735441572853	0.2814330593998752	0.3914361037119227	T	T	T
0.1775799901804456	0.4383584768520803	0.3872403710500952	T	T	T

0.7567357779545892	0.3103455557237403	0.3927374741362482	T	T	T
0.3302160754117817	0.2272094334232058	0.4160490391241819	T	T	T
0.6834876284122039	0.0398727045796163	0.3711837941517193	T	T	T
0.8470138906324264	0.1977687190655988	0.3067277577929688	T	T	T

Figure 3a State 3 → 3-Fe' TS (NUPDOWN=8)

1.0000000000000000					
8.7372206091223994	0.0000000000000000	0.0000000000000000			
0.0000000000000000	6.9809029500783426	0.0000000000000000			
0.0000000000000000	0.0000000000000000	25.0000000000000000			
K	Ni	O	H	Fe	
4	11	36	22	1	
Selective dynamics					
Direct					
0.0000000000000000	0.9295476953180499	0.0219900692777486	F	F	F
0.5000000000000000	0.8431778700801544	0.1149178963106294	F	F	F
0.9836296339390460	0.7656679484362359	0.2126139514619278	T	T	T
0.5892527558279406	0.6665115455649379	0.3498590031340539	T	T	T
0.0000000000000000	0.4295476953180497	0.0219900692777486	F	F	F
0.3336660000000009	0.4295476953180497	0.0219900692777486	F	F	F
0.6663339999999991	0.4295476953180497	0.0219900692777486	F	F	F
0.1663339999999991	0.3431778700801547	0.1149178963106294	F	F	F
0.5000000000000000	0.3431778700801547	0.1149178963106294	F	F	F
0.8336660000000009	0.3431778700801547	0.1149178963106294	F	F	F
0.9983618286561113	0.2674164298040358	0.2095834244818081	T	T	T
0.3319492011303427	0.2593707863215474	0.2100294885253080	T	T	T
0.6675302263645199	0.2620634283214787	0.2101483814035690	T	T	T
0.1622701059432236	0.1853654077853456	0.3072151976576317	T	T	T
0.5040268094163323	0.1930578240430495	0.3075991635297351	T	T	T
0.1735150000000019	0.5955569454815901	0.0004884286588833	F	F	F
0.5000000000000000	0.5859389052830437	0.0000000000000000	F	F	F
0.8264849999999981	0.5955569454815901	0.0004884286588833	F	F	F
0.1735150000000019	0.2635384451545022	0.0434917098966210	F	F	F
0.5000000000000000	0.2731564853530558	0.0439801385555043	F	F	F
0.8264849999999981	0.2635384451545022	0.0434917098966210	F	F	F
0.0000000000000000	0.4995690800451488	0.0929278270328737	F	F	F
0.3264849999999981	0.5091871202437019	0.0934162556917641	F	F	F
0.6735150000000019	0.5091871202437019	0.0934162556917641	F	F	F
0.0000000000000000	0.1867866601151605	0.1369079655883780	F	F	F
0.3264849999999981	0.1771686199166141	0.1364195369294947	F	F	F
0.6735150000000019	0.1771686199166141	0.1364195369294947	F	F	F
0.1678960421289669	0.4204093811785625	0.1870811631002648	T	T	T
0.4995641769463968	0.4164514299803888	0.1873656712493563	T	T	T
0.8314045835712047	0.4220890306053711	0.1864394310335344	T	T	T
0.1622495252981977	0.1099621161163803	0.2334438402707875	T	T	T
0.5014233948081598	0.1031148586559253	0.2342692817744063	T	T	T
0.8329761776301317	0.1121147316400987	0.2332596435149325	T	T	T
0.9889230402078742	0.3643786382094003	0.2785633023820671	T	T	T
0.3327570170316946	0.3382692037967296	0.2823077537893248	T	T	T
0.6651881814267652	0.3479567195419485	0.2814216946116063	T	T	T
0.9885918124177955	0.0263462567920498	0.3207035476939574	T	T	T
0.3513755131245564	0.0164667198310664	0.3306466685533123	T	T	T
0.6747930118042988	0.0405779893547194	0.3311361536719422	T	T	T
0.3436370000000011	0.9295476953180499	0.0219900692777486	F	F	F
0.6563629999999989	0.9295476953180499	0.0219900692777486	F	F	F
0.1563629999999989	0.8431778700801544	0.1149178963106294	F	F	F
0.8436370000000011	0.8431778700801544	0.1149178963106294	F	F	F
0.2112949601226631	0.6944972392123321	0.2961909476585535	T	T	T
0.6172759962361051	0.7400449068699975	0.2409364534438923	T	T	T
0.2302007632130093	0.6354682372465918	0.4028356014510921	T	T	T
0.8921491600490423	0.7318038622097852	0.3909442171642006	T	T	T

0.4855251655995281	0.3146981647531569	0.3731370025617564	T	T	T
0.8476349977104830	0.3142728506748110	0.3692094015302711	T	T	T
0.1512451084439691	0.2690436892601005	0.3842292649091232	T	T	T
0.7378240985415313	0.1523560301764067	0.4238763193849666	T	T	T
0.2777910000000006	0.8194148176612188	0.0136009167645312	F	F	F
0.2777910000000006	0.0396805729748735	0.0303792217909731	F	F	F
0.7222089999999994	0.8194148176612188	0.0136009167645312	F	F	F
0.7222089999999994	0.0396805729748735	0.0303792217909731	F	F	F
0.2222089999999994	0.7330449924233309	0.1065287437974050	F	F	F
0.2222089999999994	0.9533107477369782	0.1233070488238468	F	F	F
0.7777910000000006	0.7330449924233309	0.1065287437974050	F	F	F
0.7777910000000006	0.9533107477369782	0.1233070488238468	F	F	F
0.2712989202643333	0.5796346445647362	0.2858737624625405	T	T	T
0.2800615054479572	0.8065279145168552	0.2984599664246778	T	T	T
0.5620228001890536	0.6377890927493025	0.2218405173355068	T	T	T
0.5629606766293099	0.8628625522258506	0.2357069368061196	T	T	T
0.2131253824218797	0.6671014049933039	0.3640577070099392	T	T	T
0.1409874894051381	0.6909794004011958	0.4207413696126732	T	T	T
0.9033956718816242	0.5981107722102281	0.3794719143564156	T	T	T
0.9349498821641512	0.8132596604556430	0.3621852890832029	T	T	T
0.3438011802694651	0.0452249738986595	0.3691192781375326	T	T	T
0.0379110831781822	0.2848588962529383	0.3882667714292760	T	T	T
0.1970826251574747	0.3989163554563958	0.3930335684538658	T	T	T
0.8285262959185345	0.0826603809292690	0.4361310081815007	T	T	T
0.5674739508472484	0.2727126478169440	0.3974577161595340	T	T	T
0.6917475733415746	0.0672364455602701	0.3725305534228793	T	T	T
0.8447788944265063	0.1984738463011599	0.3081384832285852	T	T	T

Figure 3a State 3-Fe' (NUPDOWN=8)

```

1.0000000000000000
8.7372206091223994    0.0000000000000000    0.0000000000000000
0.0000000000000000    6.9809029500783426    0.0000000000000000
0.0000000000000000    0.0000000000000000    25.0000000000000000

```

```

K      Ni      O      H      Fe
4      11      36      22      1

```

Selective dynamics

Direct

0.0000000000000000	0.9295476953180497	0.0219900692777486	F	F	F
0.5000000000000000	0.8431778700801544	0.1149178963106294	F	F	F
0.9826272916763985	0.7637687804333111	0.2110192628119049	T	T	T
0.5785709253779330	0.6535590751777725	0.3443468360359797	T	T	T
0.0000000000000000	0.4295476953180497	0.0219900692777486	F	F	F
0.3336660000000009	0.4295476953180497	0.0219900692777486	F	F	F
0.6663339999999991	0.4295476953180497	0.0219900692777486	F	F	F
0.1663339999999991	0.3431778700801544	0.1149178963106294	F	F	F
0.5000000000000000	0.3431778700801544	0.1149178963106294	F	F	F
0.8336660000000009	0.3431778700801544	0.1149178963106294	F	F	F
0.9990724798321753	0.2666337603092396	0.2095642010726445	T	T	T
0.3314966180657379	0.2576887988152894	0.2101241373379732	T	T	T
0.6678921637047096	0.2601604771644477	0.2101060431085424	T	T	T
0.1652517146395852	0.1827372899849970	0.3066910872822091	T	T	T
0.5053507554853888	0.1850441139298316	0.3073918195182648	T	T	T
0.1735150000000019	0.5955569454815901	0.0004884286588833	F	F	F
0.5000000000000000	0.5859389052830437	0.0000000000000000	F	F	F
0.8264849999999981	0.5955569454815901	0.0004884286588833	F	F	F
0.1735150000000019	0.2635384451545022	0.0434917098966210	F	F	F
0.5000000000000000	0.2731564853530557	0.0439801385555043	F	F	F
0.8264849999999981	0.2635384451545022	0.0434917098966210	F	F	F
0.0000000000000000	0.4995690800451484	0.0929278270328737	F	F	F
0.3264849999999981	0.5091871202437019	0.0934162556917641	F	F	F
0.6735150000000019	0.5091871202437019	0.0934162556917641	F	F	F



0.0000000000000000	0.1867866601151604	0.1369079655883780	F	F	F
0.3264849999999981	0.1771686199166140	0.1364195369294947	F	F	F
0.6735150000000019	0.1771686199166140	0.1364195369294947	F	F	F
0.1675651493588227	0.4195636117474943	0.1873556005724429	T	T	T
0.4993974708161592	0.4142760922145363	0.1875475655015690	T	T	T
0.8307237613046610	0.4213375589001132	0.1865197899970053	T	T	T
0.1635006368311743	0.1065879653937060	0.2335592371157116	T	T	T
0.5010114841096037	0.1014478901619835	0.2342132457032660	T	T	T
0.8350031704266763	0.1087150113550827	0.2327735266058413	T	T	T
0.9879453017826922	0.3613259300106936	0.2792161411712386	T	T	T
0.3322127105825904	0.3363363019115868	0.2827387413986925	T	T	T
0.6684728109338689	0.3417513031182562	0.2823382043533346	T	T	T
0.9924630672427548	0.0297259795473696	0.3227286540220676	T	T	T
0.3498844350577467	0.0071583231852002	0.3289208100726255	T	T	T
0.6791423808705623	0.0238734700843644	0.3299919757876851	T	T	T
0.3436370000000011	0.9295476953180497	0.0219900692777486	F	F	F
0.6563629999999989	0.9295476953180497	0.0219900692777486	F	F	F
0.1563629999999989	0.8431778700801544	0.1149178963106294	F	F	F
0.8436370000000011	0.8431778700801544	0.1149178963106294	F	F	F
0.2002429768499301	0.6901018214307377	0.2963920399388093	T	T	T
0.6122154287875453	0.7379899772070523	0.2380413546225902	T	T	T
0.2423476654558130	0.6399557675216535	0.4017161344982070	T	T	T
0.8822474960341490	0.7450787771841890	0.3939782266658872	T	T	T
0.4907113655767003	0.2953932057948488	0.3748943348163893	T	T	T
0.8565604692025560	0.3224398189571246	0.3738530458797922	T	T	T
0.1568040718586218	0.2731495038809160	0.3826790150937143	T	T	T
0.7950112020342244	0.2103714996830074	0.4190827061412623	T	T	T
0.2777910000000006	0.8194148176612188	0.0136009167645312	F	F	F
0.2777910000000006	0.0396805729748735	0.0303792217909731	F	F	F
0.7222089999999994	0.8194148176612188	0.0136009167645312	F	F	F
0.7222089999999994	0.0396805729748735	0.0303792217909731	F	F	F
0.2222089999999994	0.7330449924233307	0.1065287437974050	F	F	F
0.2222089999999994	0.9533107477369782	0.1233070488238468	F	F	F
0.7777910000000006	0.7330449924233307	0.1065287437974050	F	F	F
0.7777910000000006	0.9533107477369782	0.1233070488238468	F	F	F
0.2594528530927576	0.5752959573289630	0.2854297223234816	T	T	T
0.2690714391596311	0.8025868261656961	0.2972739826107039	T	T	T
0.5569217189930872	0.6352846727752043	0.2189862467033174	T	T	T
0.5570744403381797	0.8608234274553488	0.2337602691401451	T	T	T
0.2123970445839080	0.6695488407465164	0.3636633123464827	T	T	T
0.1593813901968664	0.6928562181074247	0.4233120916257033	T	T	T
0.8917477231816904	0.6075778091671907	0.3863829890331041	T	T	T
0.9297751127239808	0.8140869255534523	0.3636735923187679	T	T	T
0.3441034401405088	0.0292212302311892	0.3677280683500349	T	T	T
0.0448010375722066	0.3060293425847416	0.3845420509796127	T	T	T
0.2121788587124073	0.3959598256392314	0.3911433063662610	T	T	T
0.8746499424102145	0.1121496721970347	0.4246583821778659	T	T	T
0.5810612714086200	0.2629993675597215	0.3962756609838409	T	T	T
0.6877953036966903	0.0398519746661530	0.3690645167340942	T	T	T
0.8461885295975582	0.1935080451117904	0.3059100004408151	T	T	T

Figure 3a State 4 (NUPDOWN=9)

1.0000000000000000					
8.7372206091223994	0.0000000000000000	0.0000000000000000			
0.0000000000000000	6.9809029500783426	0.0000000000000000			
0.0000000000000000	0.0000000000000000	25.0000000000000000			
K	Ni	O	H	Fe	
4	11	36	21	1	
Selective dynamics					
Direct					
0.0000000000000000	0.9295476953180497	0.0219900692777486	F	F	F



0.5000000000000000	0.8431778700801544	0.1149178963106294	F	F	F
0.9842006431927097	0.7642211970987762	0.2101482993296555	T	T	T
0.5996392143611675	0.6594538936189513	0.3424891098463353	T	T	T
0.0000000000000000	0.4295476953180497	0.0219900692777486	F	F	F
0.3336660000000009	0.4295476953180497	0.0219900692777486	F	F	F
0.6663339999999991	0.4295476953180497	0.0219900692777486	F	F	F
0.1663339999999991	0.3431778700801544	0.1149178963106294	F	F	F
0.5000000000000000	0.3431778700801544	0.1149178963106294	F	F	F
0.8336660000000009	0.3431778700801544	0.1149178963106294	F	F	F
0.9987189632511588	0.2661619530495899	0.2096343318137883	T	T	T
0.3316424583564950	0.2570282872956857	0.2102417421375795	T	T	T
0.6673305313163392	0.2592741928958057	0.2101333377680169	T	T	T
0.1641184593598460	0.1829566009817255	0.3070096589451838	T	T	T
0.5055172711629301	0.1809179758225927	0.3079699967651228	T	T	T
0.1735150000000019	0.5955569454815901	0.0004884286588833	F	F	F
0.5000000000000000	0.5859389052830437	0.0000000000000000	F	F	F
0.8264849999999998	0.5955569454815901	0.0004884286588833	F	F	F
0.1735150000000019	0.2635384451545022	0.0434917098966210	F	F	F
0.5000000000000000	0.2731564853530557	0.0439801385555043	F	F	F
0.8264849999999998	0.2635384451545022	0.0434917098966210	F	F	F
0.0000000000000000	0.4995690800451484	0.0929278270328737	F	F	F
0.3264849999999998	0.5091871202437019	0.0934162556917641	F	F	F
0.6735150000000019	0.5091871202437019	0.0934162556917641	F	F	F
0.0000000000000000	0.1867866601151604	0.1369079655883780	F	F	F
0.3264849999999998	0.1771686199166140	0.1364195369294947	F	F	F
0.6735150000000019	0.1771686199166140	0.1364195369294947	F	F	F
0.1677095963481125	0.4190399936664717	0.1873512980618256	T	T	T
0.4993518170494282	0.4139943808535683	0.1875244609446878	T	T	T
0.8305387496888682	0.4209691590614694	0.1866268129491635	T	T	T
0.1634880958629271	0.1070641304358012	0.2339860584555201	T	T	T
0.5006474947892489	0.0995141191489402	0.2329708285456109	T	T	T
0.8340644218599461	0.1090856549014917	0.2337613915590974	T	T	T
0.9885924950685586	0.3622626285272343	0.2787087822953492	T	T	T
0.3340054248803765	0.3332233748021995	0.2836993160680248	T	T	T
0.6652279658048872	0.3411280668365039	0.2823567279723972	T	T	T
0.9913877707114003	0.0317218779317131	0.3221634515677063	T	T	T
0.3511342288448507	0.0003644023224282	0.3283605020990445	T	T	T
0.6817302097999306	0.0288498161552226	0.3325889147356664	T	T	T
0.3436370000000011	0.9295476953180497	0.0219900692777486	F	F	F
0.6563629999999998	0.9295476953180497	0.0219900692777486	F	F	F
0.1563629999999998	0.8431778700801544	0.1149178963106294	F	F	F
0.8436370000000011	0.8431778700801544	0.1149178963106294	F	F	F
0.2088056514478350	0.6919069108080095	0.2885937723926120	T	T	T
0.6138328827596422	0.7390755653975236	0.2369238972740682	T	T	T
0.2204804724767613	0.6428070805254862	0.3952086322455196	T	T	T
0.8927066167635201	0.7274883301174897	0.3919202010549477	T	T	T
0.4973506999547278	0.3002082189038919	0.3767389635405135	T	T	T
0.8570014183161818	0.3356157090464597	0.3726332740168014	T	T	T
0.1550568346276937	0.2715151607963027	0.3823143510253951	T	T	T
0.5647036037942386	0.2141846839771986	0.4167982278007482	T	T	T
0.2777910000000006	0.8194148176612188	0.0136009167645312	F	F	F
0.2777910000000006	0.0396805729748735	0.0303792217909731	F	F	F
0.7222089999999994	0.8194148176612188	0.0136009167645312	F	F	F
0.7222089999999994	0.0396805729748735	0.0303792217909731	F	F	F
0.2222089999999994	0.7330449924233307	0.1065287437974050	F	F	F
0.2222089999999994	0.9533107477369782	0.1233070488238468	F	F	F
0.7777910000000006	0.7330449924233307	0.1065287437974050	F	F	F
0.7777910000000006	0.9533107477369782	0.1233070488238468	F	F	F
0.2682485885933575	0.5742045950040701	0.2807573039566947	T	T	T
0.2796426361824290	0.8017893600876702	0.2920777693661778	T	T	T
0.5582448127484418	0.6348483001547199	0.2185827558770166	T	T	T

0.5575770416900527	0.8612704724181350	0.2324514160698048	T	T	T
0.2039477157321325	0.6692060189961085	0.3560234245901632	T	T	T
0.1248989652396154	0.6886497024726345	0.4116900749698272	T	T	T
0.8962429964515110	0.5933269238178417	0.3789712187705416	T	T	T
0.9310263592657178	0.8120718110583366	0.3632269200080833	T	T	T
0.3372989223203340	-0.0042322161552508	0.3672558271827520	T	T	T
0.0402935240454333	0.2850804214415660	0.3868371673308995	T	T	T
0.1947181215354104	0.4067394086985041	0.3883930451340040	T	T	T
0.7838576414439009	0.2897946574334223	0.3995950296116661	T	T	T
0.6751265900149522	0.0492105308969849	0.3717537405040640	T	T	T
0.8460883451896167	0.1977954481060714	0.3066887665100685	T	T	T

Figure 3a State 5 (NUPDOWN=9)

1.0000000000000000		
8.7372206091223994	0.0000000000000000	0.0000000000000000
0.0000000000000000	6.9809029500783426	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000

K	Ni	O	H	Fe
4	11	34	21	1

Selective dynamics

Direct

0.0000000000000000	0.9295476953180497	0.0219900692777486	F	F	F
0.5000000000000000	0.8431778700801544	0.1149178963106294	F	F	F
0.9905968592285422	0.7643222772907692	0.2094142123240033	T	T	T
0.6249066717063044	0.6535423261429490	0.3425280198314626	T	T	T
0.0000000000000000	0.4295476953180497	0.0219900692777486	F	F	F
0.3336660000000000	0.4295476953180497	0.0219900692777486	F	F	F
0.6663339999999991	0.4295476953180497	0.0219900692777486	F	F	F
0.1663339999999991	0.3431778700801544	0.1149178963106294	F	F	F
0.5000000000000000	0.3431778700801544	0.1149178963106294	F	F	F
0.8336660000000000	0.3431778700801544	0.1149178963106294	F	F	F
0.9990722124321706	0.2649406807811226	0.2100745081252124	T	T	T
0.3333027430601140	0.2549943782573332	0.2098612269656247	T	T	T
0.6676120243316429	0.2575032696577568	0.2099218100615572	T	T	T
0.1654620560855499	0.1843431574090218	0.3080076465939067	T	T	T
0.5064210906315709	0.1763227200372395	0.3068091477543640	T	T	T
0.1735150000000019	0.5955569454815901	0.0004884286588833	F	F	F
0.5000000000000000	0.5859389052830437	0.0000000000000000	F	F	F
0.8264849999999981	0.5955569454815901	0.0004884286588833	F	F	F
0.1735150000000019	0.2635384451545022	0.0434917098966210	F	F	F
0.5000000000000000	0.2731564853530557	0.0439801385555043	F	F	F
0.8264849999999981	0.2635384451545022	0.0434917098966210	F	F	F
0.0000000000000000	0.4995690800451484	0.0929278270328737	F	F	F
0.3264849999999981	0.5091871202437019	0.0934162556917641	F	F	F
0.6735150000000019	0.5091871202437019	0.0934162556917641	F	F	F
0.0000000000000000	0.1867866601151604	0.1369079655883780	F	F	F
0.3264849999999981	0.1771686199166140	0.1364195369294947	F	F	F
0.6735150000000019	0.1771686199166140	0.1364195369294947	F	F	F
0.1680396352801314	0.4172957602421083	0.1878239499224166	T	T	T
0.5012277624784323	0.4140834133304272	0.1872713223593572	T	T	T
0.8305886765117293	0.4198119912367272	0.1870623356219605	T	T	T
0.1634751736359980	0.1062952089050519	0.2351286139764125	T	T	T
0.5014059915190823	0.0939212916055178	0.2285505312438763	T	T	T
0.8344935952558531	0.1076760199990558	0.2351885212736393	T	T	T
0.9874472893397819	0.3635803828803968	0.2790202245251753	T	T	T
0.3415673122038539	0.3293682990291069	0.2836743068602407	T	T	T
0.6627516299820254	0.3377509202854103	0.2828506048317926	T	T	T
0.9892097699547161	0.0369469320641698	0.3254554673105436	T	T	T
0.3519279124931293	0.0076410738422235	0.3310900327070681	T	T	T
0.6764984875545321	0.0378968745576113	0.3379596263464277	T	T	T
0.3436370000000011	0.9295476953180497	0.0219900692777486	F	F	F

0.6563629999999999	0.9295476953180497	0.0219900692777486	F	F	F
0.1563629999999999	0.8431778700801544	0.1149178963106294	F	F	F
0.8436370000000011	0.8431778700801544	0.1149178963106294	F	F	F
0.2221030594539495	0.6900915919409093	0.2905730281889990	T	T	T
0.6061532209515451	0.7354366588986423	0.2408563368044598	T	T	T
0.2466602445674485	0.6452148978622230	0.3961866198277547	T	T	T
0.9234701165471629	0.7442285109212470	0.3979748557819708	T	T	T
0.8555591349114823	0.3525899041006180	0.3737622359063846	T	T	T
0.1585468444615528	0.2826982911550172	0.3831650399941937	T	T	T
0.2777910000000006	0.8194148176612188	0.0136009167645312	F	F	F
0.2777910000000006	0.0396805729748735	0.0303792217909731	F	F	F
0.7222089999999994	0.8194148176612188	0.0136009167645312	F	F	F
0.7222089999999994	0.0396805729748735	0.0303792217909731	F	F	F
0.2222089999999994	0.7330449924233307	0.1065287437974050	F	F	F
0.2222089999999994	0.9533107477369782	0.1233070488238468	F	F	F
0.7777910000000006	0.7330449924233307	0.1065287437974050	F	F	F
0.7777910000000006	0.9533107477369782	0.1233070488238468	F	F	F
0.2821250094072617	0.5751686117896143	0.2804318904103046	T	T	T
0.2905934480266393	0.8025625079293623	0.2922397771238868	T	T	T
0.5576758385800669	0.6314643480517236	0.2200544383002773	T	T	T
0.5555338713616339	0.8590656644395308	0.2325821852123031	T	T	T
0.2302094244728164	0.6689498859517129	0.3566148863256418	T	T	T
0.1510689054150509	0.6948067551303900	0.4120412628343803	T	T	T
0.9170909274401682	0.6127022316780397	0.3835968398076175	T	T	T
0.9511114629134284	0.8323730983702144	0.3682694501630151	T	T	T
0.3417700421286317	-0.0044026154111267	0.3699116794336935	T	T	T
0.0443528757471559	0.3039214499441296	0.3860182164387865	T	T	T
0.2034431062238564	0.4153017768619836	0.3888102430217434	T	T	T
0.8086895490515874	0.2880607059988693	0.4042776955575589	T	T	T
0.6772691479505093	0.0541046722763563	0.3768113341774331	T	T	T
0.8464719166771336	0.2024692273462603	0.3077003948137987	T	T	T

Figure 3b State 1 (NUPDOWN=12)

1.000000000000000		
8.7372206091223994	0.0000000000000000	0.0000000000000000
0.0000000000000000	6.9809029500783426	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000

K	Ni	O	H	Fe
4	10	34	20	2

Selective dynamics

Direct

0.0000000000000000	0.9295476953180497	0.0219900692777486	F	F	F
0.5000000000000000	0.8431778700801544	0.1149178963106294	F	F	F
0.9889514477874014	0.7588329958936809	0.2123468977539028	T	T	T
0.6120133026063541	0.6740654276456028	0.3473613323746633	T	T	T
0.0000000000000000	0.4295476953180497	0.0219900692777486	F	F	F
0.3336660000000009	0.4295476953180497	0.0219900692777486	F	F	F
0.6663339999999991	0.4295476953180497	0.0219900692777486	F	F	F
0.1663339999999991	0.3431778700801544	0.1149178963106294	F	F	F
0.5000000000000000	0.3431778700801544	0.1149178963106294	F	F	F
0.8336660000000009	0.3431778700801544	0.1149178963106294	F	F	F
-0.0007267475864841	0.2599793194952466	0.2102147225475084	T	T	T
0.6675456575897080	0.2571671994535271	0.2097104142917621	T	T	T
0.1634406407801873	0.1772559474684013	0.3083004203757932	T	T	T
0.5116103737429690	0.1818720933920230	0.3057799211307110	T	T	T
0.1735150000000019	0.5955569454815901	0.0004884286588833	F	F	F
0.5000000000000000	0.5859389052830437	0.0000000000000000	F	F	F
0.8264849999999981	0.5955569454815901	0.0004884286588833	F	F	F
0.1735150000000019	0.2635384451545022	0.0434917098966210	F	F	F
0.5000000000000000	0.2731564853530557	0.0439801385555043	F	F	F
0.8264849999999981	0.2635384451545022	0.0434917098966210	F	F	F

0.0000000000000000	0.4995690800451484	0.0929278270328737	F	F	F
0.3264849999999981	0.5091871202437019	0.0934162556917641	F	F	F
0.6735150000000019	0.5091871202437019	0.0934162556917641	F	F	F
0.0000000000000000	0.1867866601151604	0.1369079655883780	F	F	F
0.3264849999999981	0.1771686199166140	0.1364195369294947	F	F	F
0.6735150000000019	0.1771686199166140	0.1364195369294947	F	F	F
0.1673477719977688	0.4160391481917738	0.1882942428627315	T	T	T
0.4997853862481418	0.4153897443806611	0.1876739555127340	T	T	T
0.8327760148396984	0.4172541397461440	0.1875915194281954	T	T	T
0.1666088601638418	0.0996358675619548	0.2301855128769250	T	T	T
0.4986207555461355	0.0917565090749173	0.2255620538360684	T	T	T
0.8322262254396028	0.1028854517404206	0.2339824659882955	T	T	T
0.9918025198533648	0.3455583384290954	0.2807108780129539	T	T	T
0.3467632707200775	0.3392152938846074	0.2811829589563309	T	T	T
0.6645967554912383	0.3421418104002123	0.2813157395520663	T	T	T
0.9797572579555509	0.0140778826446534	0.3250448475897084	T	T	T
0.3548028943779230	0.0147150584657730	0.3307546316622997	T	T	T
0.6731964364484839	0.0504219506363399	0.3321809233881190	T	T	T
0.3436370000000011	0.9295476953180497	0.0219900692777486	F	F	F
0.6563629999999989	0.9295476953180497	0.0219900692777486	F	F	F
0.1563629999999989	0.8431778700801544	0.1149178963106294	F	F	F
0.8436370000000011	0.8431778700801544	0.1149178963106294	F	F	F
0.2206890430570346	0.6909696042680814	0.2924918486486745	T	T	T
0.6158915040999058	0.7352213976688059	0.2416622031944620	T	T	T
0.2311796678007699	0.6369386753789870	0.3988087514853121	T	T	T
0.9038968862356223	0.7216798596811649	0.3964988160497069	T	T	T
0.8492703395216500	0.3277242460131335	0.3738798155763249	T	T	T
0.1540634240140142	0.2686768366539026	0.3866532254974037	T	T	T
0.2777910000000006	0.8194148176612188	0.0136009167645312	F	F	F
0.2777910000000006	0.0396805729748735	0.0303792217909731	F	F	F
0.7222089999999994	0.8194148176612188	0.0136009167645312	F	F	F
0.7222089999999994	0.0396805729748735	0.0303792217909731	F	F	F
0.2222089999999994	0.7330449924233307	0.1065287437974050	F	F	F
0.2222089999999994	0.9533107477369782	0.1233070488238468	F	F	F
0.7777910000000006	0.7330449924233307	0.1065287437974050	F	F	F
0.7777910000000006	0.9533107477369782	0.1233070488238468	F	F	F
0.2810931882116395	0.5753546433267263	0.2827862672279747	T	T	T
0.2897010341695924	0.8026829042177588	0.2955739581350053	T	T	T
0.5646298203966886	0.6305540047919177	0.2221135629729514	T	T	T
0.5634683741016043	0.8571334614091011	0.2333035323581409	T	T	T
0.2178704625965082	0.6627991936284816	0.3594003434442616	T	T	T
0.1344658261895730	0.6850555307326500	0.4140954474057692	T	T	T
0.9055104258044853	0.5907674203502692	0.3816900937691652	T	T	T
0.9343524335814508	0.8129313273671667	0.3678521632945168	T	T	T
0.3457262443617304	0.0096576442076710	0.3697331165640492	T	T	T
0.7870883673943595	0.2578531499687763	0.3998563041152149	T	T	T
0.0399144749354477	0.2818007670569291	0.3898999798278863	T	T	T
0.1932781340260015	0.4034056483063168	0.3928694612070318	T	T	T
0.3334860144228914	0.2513862874120399	0.2109650895175080	T	T	T
0.8389061394579912	0.1823599578976192	0.3088016925525232	T	T	T

Figure 3b State 2 (NUPDOWN=11)

1.0000000000000000					
8.7372206091223994	0.0000000000000000	0.0000000000000000			
0.0000000000000000	6.9809029500783426	0.0000000000000000			
0.0000000000000000	0.0000000000000000	25.0000000000000000			
K	Ni	O	H	Fe	
4	10	35	21	2	
Selective dynamics					
Direct					
0.0000000000000000	0.9295476953180497	0.0219900692777486	F	F	F

0.5000000000000000	0.8431778700801544	0.1149178963106294	F	F	F
0.0417464980832278	0.7613097152813831	0.2076645472371570	T	T	T
0.5315674838787685	0.6831340171347861	0.3457603872028255	T	T	T
0.0000000000000000	0.4295476953180497	0.0219900692777486	F	F	F
0.3336660000000009	0.4295476953180497	0.0219900692777486	F	F	F
0.6663339999999991	0.4295476953180497	0.0219900692777486	F	F	F
0.1663339999999991	0.3431778700801544	0.1149178963106294	F	F	F
0.5000000000000000	0.3431778700801544	0.1149178963106294	F	F	F
0.8336660000000009	0.3431778700801544	0.1149178963106294	F	F	F
0.9984136425734429	0.2638236115590692	0.2096066186623633	T	T	T
0.6657403184263544	0.2581243711779053	0.2096818102078346	T	T	T
0.1652799136461481	0.1809023570770262	0.3060551086363418	T	T	T
0.5094655532784063	0.1880170835288665	0.3070835711590697	T	T	T
0.1735150000000019	0.5955569454815901	0.0004884286588833	F	F	F
0.5000000000000000	0.5859389052830437	0.0000000000000000	F	F	F
0.8264849999999981	0.5955569454815901	0.0004884286588833	F	F	F
0.1735150000000019	0.2635384451545022	0.0434917098966210	F	F	F
0.5000000000000000	0.2731564853530557	0.0439801385555043	F	F	F
0.8264849999999981	0.2635384451545022	0.0434917098966210	F	F	F
0.0000000000000000	0.4995690800451484	0.0929278270328737	F	F	F
0.3264849999999981	0.5091871202437019	0.0934162556917641	F	F	F
0.6735150000000019	0.5091871202437019	0.0934162556917641	F	F	F
0.0000000000000000	0.1867866601151604	0.1369079655883780	F	F	F
0.3264849999999981	0.1771686199166140	0.1364195369294947	F	F	F
0.6735150000000019	0.1771686199166140	0.1364195369294947	F	F	F
0.1673769036619566	0.4173548512503411	0.1878203377853516	T	T	T
0.4981728623198539	0.4150987105067346	0.1884716393753267	T	T	T
0.8301358548436268	0.4226387935895277	0.1868142981068173	T	T	T
0.1628982723101981	0.1042124927834023	0.2327248032398999	T	T	T
0.4991234944604906	0.0956279984716022	0.2330141326099024	T	T	T
0.8313933033349163	0.1038694997518860	0.2328211221271999	T	T	T
0.9869399382610528	0.3576902428183591	0.2788235291425001	T	T	T
0.3347127609506606	0.3322443251565904	0.2817818670186540	T	T	T
0.6654464093796844	0.3472345632765244	0.2807535326587806	T	T	T
0.9918417858127172	0.0341911150107649	0.3226625292611698	T	T	T
0.3579015041791599	0.0209450206015645	0.3342686598903371	T	T	T
0.6802833795386249	0.0408290414104587	0.3260251176344385	T	T	T
0.3436370000000011	0.9295476953180497	0.0219900692777486	F	F	F
0.6563629999999989	0.9295476953180497	0.0219900692777486	F	F	F
0.1563629999999989	0.8431778700801544	0.1149178963106294	F	F	F
0.8436370000000011	0.8431778700801544	0.1149178963106294	F	F	F
0.3568851564550938	0.7314729797579078	0.2469409739132347	T	T	T
0.7319593888586045	0.7307617649593598	0.2512530309104887	T	T	T
0.1959116710867743	0.6470190153012854	0.3503652210600984	T	T	T
0.8723760426420821	0.6946844954918741	0.3479508574135116	T	T	T
0.5130214678320727	0.3048445087061913	0.3736448929995563	T	T	T
0.8478751984870320	0.3154523966051754	0.3743139310937609	T	T	T
0.1553412678741684	0.2880872993546148	0.3786900799181742	T	T	T
0.2777910000000006	0.8194148176612188	0.0136009167645312	F	F	F
0.2777910000000006	0.0396805729748735	0.0303792217909731	F	F	F
0.7222089999999994	0.8194148176612188	0.0136009167645312	F	F	F
0.7222089999999994	0.0396805729748735	0.0303792217909731	F	F	F
0.2222089999999994	0.7330449924233307	0.1065287437974050	F	F	F
0.2222089999999994	0.9533107477369782	0.1233070488238468	F	F	F
0.7777910000000006	0.7330449924233307	0.1065287437974050	F	F	F
0.7777910000000006	0.9533107477369782	0.1233070488238468	F	F	F
0.4175388587661500	0.6316352615400537	0.2289074733425981	T	T	T
0.4146665770017087	0.8524531094731440	0.2433353941607224	T	T	T
0.7522060942165114	0.6349928946961424	0.2230438966511472	T	T	T
0.7520461589358544	0.8613632040730487	0.2375628213425042	T	T	T
0.2360626295436261	0.6606084232911773	0.3137310523121748	T	T	T

0.0847547411577077	0.6738301770435202	0.3474117527458348	T	T	T
0.8336929914239928	0.6975364725887450	0.3102397105668629	T	T	T
0.8949824084484743	0.8307840867782452	0.3552232343246702	T	T	T
0.6198152728255857	0.2837471012236800	0.3855614227574548	T	T	T
0.3535645597747263	0.0698355618198504	0.3712736664593914	T	T	T
0.0405149780713599	0.2900215699933607	0.3849762486401399	T	T	T
0.8522943948322662	0.4552060874434075	0.3670761189261257	T	T	T
0.1837888243008375	0.4273661613615505	0.3714052064720878	T	T	T
0.3325173327965957	0.2552143715805416	0.2099936046508651	T	T	T
0.8378611883644530	0.1896181189278449	0.3077909013294637	T	T	T

Figure 3b State 3 (NUPDOWN=12)

1.0000000000000000		
8.7372206091223994	0.0000000000000000	0.0000000000000000
0.0000000000000000	6.9809029500783426	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000

K	Ni	O	H	Fe
4	10	36	22	2

Selective dynamics

Direct

0.0000000000000000	0.9295476953180497	0.0219900692777486	F	F	F
0.5000000000000000	0.8431778700801544	0.1149178963106294	F	F	F
0.9836218266600358	0.7655812025421163	0.2109506065711066	T	T	T
0.5482986828787856	0.7308149240213149	0.3927290281306267	T	T	T
0.0000000000000000	0.4295476953180497	0.0219900692777486	F	F	F
0.3336660000000009	0.4295476953180497	0.0219900692777486	F	F	F
0.6663339999999991	0.4295476953180497	0.0219900692777486	F	F	F
0.1663339999999991	0.3431778700801544	0.1149178963106294	F	F	F
0.5000000000000000	0.3431778700801544	0.1149178963106294	F	F	F
0.8336660000000009	0.3431778700801544	0.1149178963106294	F	F	F
0.9975638153491330	0.2621877313990770	0.2100936018877780	T	T	T
0.6681749575292339	0.2607664337486202	0.2092748229596903	T	T	T
0.1559467785379247	0.1916754504063463	0.3071048030482069	T	T	T
0.5040368506882373	0.2078094337605756	0.3054466406523744	T	T	T
0.1735150000000019	0.5955569454815901	0.0004884286588833	F	F	F
0.5000000000000000	0.5859389052830437	0.0000000000000000	F	F	F
0.8264849999999981	0.5955569454815901	0.0004884286588833	F	F	F
0.1735150000000019	0.2635384451545022	0.0434917098966210	F	F	F
0.5000000000000000	0.2731564853530557	0.0439801385555043	F	F	F
0.8264849999999981	0.2635384451545022	0.0434917098966210	F	F	F
0.0000000000000000	0.4995690800451484	0.0929278270328737	F	F	F
0.3264849999999981	0.5091871202437019	0.0934162556917641	F	F	F
0.6735150000000019	0.5091871202437019	0.0934162556917641	F	F	F
0.0000000000000000	0.1867866601151604	0.1369079655883780	F	F	F
0.3264849999999981	0.1771686199166140	0.1364195369294947	F	F	F
0.6735150000000019	0.1771686199166140	0.1364195369294947	F	F	F
0.1655999489637454	0.4219935279735054	0.1872421305736298	T	T	T
0.4987105609936549	0.4176701003712398	0.1862508734916559	T	T	T
0.8338164486950290	0.4176532578381296	0.1869523350254867	T	T	T
0.1680081006576237	0.1115594615500953	0.2346360751322605	T	T	T
0.4967656105343096	0.1105106340361506	0.2333626927174627	T	T	T
0.8314602758957410	0.1071992443649163	0.2320408972016598	T	T	T
0.9936979516731347	0.3397384728940790	0.2820388229141059	T	T	T
0.3417320627195142	0.3655903679454306	0.2779855667042593	T	T	T
0.6662371166754830	0.3535244197898236	0.2794768512955390	T	T	T
0.9646653509988534	0.0029677906788063	0.3228656717809106	T	T	T
0.3344626234594675	0.0456390337207404	0.3271011391581440	T	T	T
0.6581260624734288	0.0361435824012411	0.3226367691329272	T	T	T
0.3436370000000011	0.9295476953180497	0.0219900692777486	F	F	F
0.6563629999999989	0.9295476953180497	0.0219900692777486	F	F	F
0.1563629999999989	0.8431778700801544	0.1149178963106294	F	F	F



0.8436370000000011	0.8431778700801544	0.1149178963106294	F	F	F
0.2191879846308629	0.7088455866268976	0.2912418952239912	T	T	T
0.6469182861525020	0.7594077048374006	0.2178177352708566	T	T	T
0.1911303211170192	0.6365851240782648	0.3951427757664124	T	T	T
0.8687057553235823	0.7026362658355984	0.3894257786248539	T	T	T
0.5199380649991447	0.3265474247162788	0.3729493522934183	T	T	T
0.8346723708278795	0.3097934377541331	0.3695465297932656	T	T	T
0.1290722342633818	0.2759514384377870	0.3805397469416692	T	T	T
0.4056798686809560	0.0544842146677384	0.4324600963780258	T	T	T
0.2777910000000006	0.8194148176612188	0.0136009167645312	F	F	F
0.2777910000000006	0.0396805729748735	0.0303792217909731	F	F	F
0.7222089999999994	0.8194148176612188	0.0136009167645312	F	F	F
0.7222089999999994	0.0396805729748735	0.0303792217909731	F	F	F
0.2222089999999994	0.7330449924233307	0.1065287437974050	F	F	F
0.2222089999999994	0.9533107477369782	0.1233070488238468	F	F	F
0.7777910000000006	0.7330449924233307	0.1065287437974050	F	F	F
0.7777910000000006	0.9533107477369782	0.1233070488238468	F	F	F
0.2840644178793574	0.5963722339320215	0.2819752999466275	T	T	T
0.2830772102648936	0.8252013740595088	0.2935292282808797	T	T	T
0.5944344443375351	0.6393932919410508	0.2261869842292498	T	T	T
0.6145664051311063	0.8543253004624217	0.2442984141395900	T	T	T
0.1948858464823786	0.6722442287251283	0.3558611275117485	T	T	T
0.0870268072470362	0.6778033637760192	0.4058489935624457	T	T	T
0.8641497612456006	0.5744836434922127	0.3722116577855021	T	T	T
0.8966570590132975	0.7985978402255491	0.3617199981723484	T	T	T
0.4532878720543100	0.1745657818491466	0.4159435164047920	T	T	T
0.0108449710403617	0.2827866798824340	0.3827958277049641	T	T	T
0.1634287659386356	0.4161884245785876	0.3864453034719528	T	T	T
0.6337028838551481	0.3191936641412877	0.3782850673087666	T	T	T
0.3127832858661911	0.0962740452752748	0.4505395587505872	T	T	T
0.3374550021995119	0.0398980772588741	0.3673258307154793	T	T	T
0.3321725346261815	0.2671713472187861	0.2097299900384594	T	T	T
0.8285905263495552	0.1783009502761609	0.3105182965431931	T	T	T

Figure 3b State 3 → 3-Ni' TS (NUPDOWN=12)

1.000000000000000		
8.7372206091223994	0.0000000000000000	0.0000000000000000
0.0000000000000000	6.9809029500783426	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000

K Ni O H Fe

4 10 36 22 2

Selective dynamics

Direct

0.0000000000000000	0.9295476953180499	0.0219900692777486	F	F	F
0.5000000000000000	0.8431778700801544	0.1149178963106294	F	F	F
0.9849633486672010	0.7591293458869015	0.2114517457689035	T	T	T
0.5815492468363523	0.6742798475717762	0.3516094610827860	T	T	T
0.0000000000000000	0.4295476953180497	0.0219900692777486	F	F	F
0.3336660000000009	0.4295476953180497	0.0219900692777486	F	F	F
0.6663339999999991	0.4295476953180497	0.0219900692777486	F	F	F
0.1663339999999991	0.3431778700801547	0.1149178963106294	F	F	F
0.5000000000000000	0.3431778700801547	0.1149178963106294	F	F	F
0.8336660000000009	0.3431778700801547	0.1149178963106294	F	F	F
0.9984646648405753	0.2608382392892712	0.2100632780550353	T	T	T
0.6675782778845749	0.2574453130277346	0.2097167451345816	T	T	T
0.1591354288683733	0.1742968488681675	0.3088407463706711	T	T	T
0.5073542071793414	0.1801420001087900	0.3051922721741125	T	T	T
0.1735150000000019	0.5955569454815901	0.0004884286588833	F	F	F
0.5000000000000000	0.5859389052830437	0.0000000000000000	F	F	F
0.8264849999999981	0.5955569454815901	0.0004884286588833	F	F	F
0.1735150000000019	0.2635384451545022	0.0434917098966210	F	F	F



0.5000000000000000	0.2731564853530558	0.0439801385555043	F	F	F
0.8264849999999981	0.2635384451545022	0.0434917098966210	F	F	F
0.0000000000000000	0.4995690800451488	0.0929278270328737	F	F	F
0.3264849999999981	0.5091871202437019	0.0934162556917641	F	F	F
0.6735150000000019	0.5091871202437019	0.0934162556917641	F	F	F
0.0000000000000000	0.1867866601151605	0.1369079655883780	F	F	F
0.3264849999999981	0.1771686199166141	0.1364195369294947	F	F	F
0.6735150000000019	0.1771686199166141	0.1364195369294947	F	F	F
0.1654034074598829	0.4184639690546586	0.1881024844794277	T	T	T
0.5006667769176772	0.4144113350795312	0.1878970075384195	T	T	T
0.8319490093458409	0.4183836600870833	0.1872140515616983	T	T	T
0.1641343112088890	0.1020182357447717	0.2301144948441114	T	T	T
0.5004361134450226	0.0937427168980649	0.2283311142813316	T	T	T
0.8333523256889338	0.1018476780424383	0.2325336173958788	T	T	T
0.9869392903277980	0.3418135009373331	0.2817987884380934	T	T	T
0.3390588820448419	0.3356589034569333	0.2801534147622460	T	T	T
0.6659683461870364	0.3392234787889270	0.2817735096356876	T	T	T
0.9796374310159351	0.0079155946103900	0.3251565684229022	T	T	T
0.3489646440584112	0.0066241460169248	0.3274758866621227	T	T	T
0.6729696445620373	0.0289140599394452	0.3245286075315987	T	T	T
0.3436370000000011	0.9295476953180499	0.0219900692777486	F	F	F
0.6563629999999989	0.9295476953180499	0.0219900692777486	F	F	F
0.1563629999999989	0.8431778700801544	0.1149178963106294	F	F	F
0.8436370000000011	0.8431778700801544	0.1149178963106294	F	F	F
0.2148286357108036	0.6927203558413032	0.2881743350671842	T	T	T
0.6134544187791146	0.7309612710412049	0.2437687272473352	T	T	T
0.2144194912279975	0.6523538309950494	0.3939450986050087	T	T	T
0.8844595190849340	0.7177424663438244	0.3936154075013036	T	T	T
0.5008806474339883	0.2835523739613921	0.3775096962802097	T	T	T
0.8347210840590997	0.2960539264075105	0.3776154323154652	T	T	T
0.1484691367743036	0.2906452941880068	0.3857082660278833	T	T	T
0.4204221177820019	0.1436149442109939	0.4300578737425536	T	T	T
0.2777910000000006	0.8194148176612188	0.0136009167645312	F	F	F
0.2777910000000006	0.0396805729748735	0.0303792217909731	F	F	F
0.7222089999999994	0.8194148176612188	0.0136009167645312	F	F	F
0.7222089999999994	0.0396805729748735	0.0303792217909731	F	F	F
0.2222089999999994	0.7330449924233309	0.1065287437974050	F	F	F
0.2222089999999994	0.9533107477369782	0.1233070488238468	F	F	F
0.7777910000000006	0.7330449924233309	0.1065287437974050	F	F	F
0.7777910000000006	0.9533107477369782	0.1233070488238468	F	F	F
0.2753482910115249	0.5761446423606077	0.2800235853772355	T	T	T
0.2846890421626397	0.8038328080724596	0.2919440996297592	T	T	T
0.5632692115783541	0.6298196949992183	0.2225608183186120	T	T	T
0.5643564900675702	0.8551634934008973	0.2356934036909896	T	T	T
0.2022068557737000	0.6782925015869634	0.3543811057492476	T	T	T
0.1197137364989901	0.7030339725471042	0.4098555962731258	T	T	T
0.8923915523850735	0.5853830937210164	0.3806758426091883	T	T	T
0.9186349546112660	0.8045472248249363	0.3644036118873658	T	T	T
0.3580743760703171	0.0092736141696430	0.3671327803915803	T	T	T
0.0342004474217581	0.2950272615729487	0.3889299188098143	T	T	T
0.1809930009889912	0.4318975447205409	0.3889050422465083	T	T	T
0.8301536726577946	0.1922044949755725	0.4038729525767145	T	T	T
0.3175275609895509	0.2029288153872650	0.4261206447098965	T	T	T
0.6089119233208081	0.2665318148850215	0.3892857911879963	T	T	T
0.3308787540382052	0.2541717566589497	0.2105566026594387	T	T	T
0.8358769132321116	0.1712808638728214	0.3074096450157368	T	T	T

Figure 3b State 3-Ni' (NUPDOWN=12)

1.0000000000000000		
8.7372206091223994	0.0000000000000000	0.0000000000000000
0.0000000000000000	6.9809029500783426	0.0000000000000000

0.0000000000000000	0.0000000000000000	25.0000000000000000			
K	Ni	O	H	Fe	
4	10	36	22	2	
Selective dynamics					
Direct					
0.0000000000000000	0.9295476953180497	0.0219900692777486	F	F	F
0.5000000000000000	0.8431778700801544	0.1149178963106294	F	F	F
0.9858288604213934	0.7633274847651513	0.2091574689216764	T	T	T
0.5870651374376263	0.6530715629728205	0.3420007136454363	T	T	T
0.0000000000000000	0.4295476953180497	0.0219900692777486	F	F	F
0.3336660000000009	0.4295476953180497	0.0219900692777486	F	F	F
0.6663339999999991	0.4295476953180497	0.0219900692777486	F	F	F
0.1663339999999991	0.3431778700801544	0.1149178963106294	F	F	F
0.5000000000000000	0.3431778700801544	0.1149178963106294	F	F	F
0.8336660000000009	0.3431778700801544	0.1149178963106294	F	F	F
0.0007813263841663	0.2638946191599682	0.2094635253365980	T	T	T
0.6695076591954101	0.2578007299540710	0.2101450387946125	T	T	T
0.1615730172780240	0.1840189537113956	0.3085601431714380	T	T	T
0.5065327058673010	0.1826187119784540	0.3071597406996266	T	T	T
0.1735150000000019	0.5955569454815901	0.0004884286588833	F	F	F
0.5000000000000000	0.5859389052830437	0.0000000000000000	F	F	F
0.8264849999999981	0.5955569454815901	0.0004884286588833	F	F	F
0.1735150000000019	0.2635384451545022	0.0434917098966210	F	F	F
0.5000000000000000	0.2731564853530557	0.0439801385555043	F	F	F
0.8264849999999981	0.2635384451545022	0.0434917098966210	F	F	F
0.0000000000000000	0.4995690800451484	0.0929278270328737	F	F	F
0.3264849999999981	0.5091871202437019	0.0934162556917641	F	F	F
0.6735150000000019	0.5091871202437019	0.0934162556917641	F	F	F
0.0000000000000000	0.1867866601151604	0.1369079655883780	F	F	F
0.3264849999999981	0.1771686199166140	0.1364195369294947	F	F	F
0.6735150000000019	0.1771686199166140	0.1364195369294947	F	F	F
0.1682221199481535	0.4194481064787459	0.1876534543554318	T	T	T
0.4999397224673328	0.4127304033225420	0.1875428723193931	T	T	T
0.8315021758871188	0.4192410208834566	0.1868998057033511	T	T	T
0.1692989588289580	0.1038079968599865	0.2303617670500359	T	T	T
0.5034255450595632	0.0960034131168429	0.2328795824475377	T	T	T
0.8364767718169644	0.1063322526194612	0.2337496667196391	T	T	T
0.9920641377860601	0.3541151162475457	0.2805501750051072	T	T	T
0.3444098976360714	0.3387254195101935	0.2810562224914948	T	T	T
0.6676620645361941	0.3397324964789575	0.2828500438815010	T	T	T
0.9836851356485444	0.0199452857002113	0.3248446313755277	T	T	T
0.3474111871360407	0.0094074393779932	0.3263253365536314	T	T	T
0.6756636214630442	0.0247487317712429	0.3312702970164485	T	T	T
0.3436370000000011	0.9295476953180497	0.0219900692777486	F	F	F
0.6563629999999989	0.9295476953180497	0.0219900692777486	F	F	F
0.1563629999999989	0.8431778700801544	0.1149178963106294	F	F	F
0.8436370000000011	0.8431778700801544	0.1149178963106294	F	F	F
0.2166437839343867	0.6931837213410285	0.2867199091482357	T	T	T
0.6171954538101174	0.7350789558942614	0.2377816530994530	T	T	T
0.2043160504294866	0.6596355978874089	0.3928146602140527	T	T	T
0.8849207317934281	0.7255238278395194	0.3910601444516756	T	T	T
0.5096778378154861	0.2979544832183510	0.3765400156942709	T	T	T
0.8500391440223963	0.3288606909985076	0.3736793666579738	T	T	T
0.1565246890841152	0.2941604978076251	0.3875818083760385	T	T	T
0.4405909517392998	0.1871061114048185	0.4179961950640183	T	T	T
0.2777910000000006	0.8194148176612188	0.0136009167645312	F	F	F
0.2777910000000006	0.0396805729748735	0.0303792217909731	F	F	F
0.7222089999999994	0.8194148176612188	0.0136009167645312	F	F	F
0.7222089999999994	0.0396805729748735	0.0303792217909731	F	F	F
0.2222089999999994	0.7330449924233307	0.1065287437974050	F	F	F
0.2222089999999994	0.9533107477369782	0.1233070488238468	F	F	F

0.7777910000000000	0.7330449924233307	0.1065287437974050	F	F	F
0.7777910000000000	0.9533107477369782	0.1233070488238468	F	F	F
0.2791718532687013	0.5778742789828584	0.2789256161623153	T	T	T
0.2840251815744971	0.8067153668141718	0.2893968938171700	T	T	T
0.5633256023909036	0.6327425995840436	0.2180364339946136	T	T	T
0.5636791454523797	0.8587060631092412	0.2326606127944364	T	T	T
0.1991173594748326	0.6802701711733994	0.3528327971726880	T	T	T
0.1036392396609587	0.7060569885427039	0.4055580583829788	T	T	T
0.8878484960851166	0.5916838934812653	0.3777001962304536	T	T	T
0.9175317977407228	0.8133764281547627	0.3619129160754586	T	T	T
0.3523054293047860	0.9948267568310549	0.3654249302760766	T	T	T
0.0444282162491486	0.2820098907324913	0.3949543527043280	T	T	T
0.1773240518955694	0.4401566646150668	0.3899103577319059	T	T	T
0.7513562991723887	0.3088376504264502	0.3916256105158348	T	T	T
0.3299005054483218	0.2274758554294808	0.4158171863995249	T	T	T
0.6775857652316216	0.0387385316973718	0.3703380692671178	T	T	T
0.3321362581109279	0.2519863304744409	0.2099431390500211	T	T	T
0.8483298745908630	0.1935257231895125	0.3070907087480155	T	T	T

Figure 3b State 3 → 3-Fe' TS (NUPDOWN=12)

1.0000000000000000					
8.7372206091223994	0.0000000000000000	0.0000000000000000			
0.0000000000000000	6.9809029500783426	0.0000000000000000			
0.0000000000000000	0.0000000000000000	25.0000000000000000			
K	Ni	O	H	Fe	
4	10	36	22	2	
Selective dynamics					
Direct					
0.0000000000000000	0.9295476953180499	0.0219900692777486	F	F	F
0.5000000000000000	0.8431778700801544	0.1149178963106294	F	F	F
0.9829479816092530	0.7653769459792156	0.2128349109276754	T	T	T
0.5905698713234583	0.6690528271597785	0.3495923646743887	T	T	T
0.0000000000000000	0.4295476953180497	0.0219900692777486	F	F	F
0.3336660000000009	0.4295476953180497	0.0219900692777486	F	F	F
0.6663339999999991	0.4295476953180497	0.0219900692777486	F	F	F
0.1663339999999991	0.3431778700801547	0.1149178963106294	F	F	F
0.5000000000000000	0.3431778700801547	0.1149178963106294	F	F	F
0.8336660000000009	0.3431778700801547	0.1149178963106294	F	F	F
0.9987601150189347	0.2654455351461777	0.2093809224347656	T	T	T
0.6684581087918167	0.2609870828488616	0.2098914666402512	T	T	T
0.1584579313656702	0.1873174228763400	0.3091984221692400	T	T	T
0.5044883410880917	0.1967991636638246	0.3071226158641296	T	T	T
0.1735150000000019	0.5955569454815901	0.0004884286588833	F	F	F
0.5000000000000000	0.5859389052830437	0.0000000000000000	F	F	F
0.8264849999999981	0.5955569454815901	0.0004884286588833	F	F	F
0.1735150000000019	0.2635384451545022	0.0434917098966210	F	F	F
0.5000000000000000	0.2731564853530558	0.0439801385555043	F	F	F
0.8264849999999981	0.2635384451545022	0.0434917098966210	F	F	F
0.0000000000000000	0.4995690800451488	0.0929278270328737	F	F	F
0.3264849999999981	0.5091871202437019	0.0934162556917641	F	F	F
0.6735150000000019	0.5091871202437019	0.0934162556917641	F	F	F
0.0000000000000000	0.1867866601151605	0.1369079655883780	F	F	F
0.3264849999999981	0.1771686199166141	0.1364195369294947	F	F	F
0.6735150000000019	0.1771686199166141	0.1364195369294947	F	F	F
0.1680655253002889	0.4214204520580440	0.1874063035236940	T	T	T
0.4988375285814481	0.4164265902124439	0.1870958697278548	T	T	T
0.8322301188073328	0.4208140931632698	0.1866689254530354	T	T	T
0.1661081883447410	0.1079557593409641	0.2305509735314827	T	T	T
0.5006769245347283	0.1023311852800094	0.2334645607728067	T	T	T
0.8336627966698597	0.1106195876113061	0.2330660552499202	T	T	T
0.9925900250225702	0.3564272451209158	0.2793808293884216	T	T	T

0.3392248087613778	0.3456071583758275	0.2795075306952953	T	T	T
0.6663560886101348	0.3481611002098170	0.2810952323832602	T	T	T
0.9792365478040954	0.0151902844817112	0.3217398888387716	T	T	T
0.3469367731802671	0.0258396629303616	0.3303398198994797	T	T	T
0.6703173503100425	0.0429608546112453	0.3312809374778336	T	T	T
0.3436370000000011	0.9295476953180499	0.0219900692777486	F	F	F
0.6563629999999989	0.9295476953180499	0.0219900692777486	F	F	F
0.1563629999999989	0.8431778700801544	0.1149178963106294	F	F	F
0.8436370000000011	0.8431778700801544	0.1149178963106294	F	F	F
0.2113146197227207	0.6964655772207842	0.2962919347202951	T	T	T
0.6198423270446533	0.7403523225001628	0.2403572437511010	T	T	T
0.2344042426990015	0.6416555217703201	0.4034547246435763	T	T	T
0.8903293814771848	0.7280498106500800	0.3913491616823548	T	T	T
0.4856788129765930	0.3201495288171659	0.3722916996481561	T	T	T
0.8450801829461344	0.3128608602394256	0.3689327386928462	T	T	T
0.1481170302409447	0.2747403690889264	0.3876584978921859	T	T	T
0.7331454564267724	0.1429190811239202	0.4234150003572795	T	T	T
0.2777910000000006	0.8194148176612188	0.0136009167645312	F	F	F
0.2777910000000006	0.0396805729748735	0.0303792217909731	F	F	F
0.7222089999999994	0.8194148176612188	0.0136009167645312	F	F	F
0.7222089999999994	0.0396805729748735	0.0303792217909731	F	F	F
0.2222089999999994	0.7330449924233309	0.1065287437974050	F	F	F
0.2222089999999994	0.9533107477369782	0.1233070488238468	F	F	F
0.7777910000000006	0.7330449924233309	0.1065287437974050	F	F	F
0.7777910000000006	0.9533107477369782	0.1233070488238468	F	F	F
0.2733268099500865	0.5836044633651816	0.2857141604486097	T	T	T
0.2781252434079674	0.8102955306742382	0.2983164732408991	T	T	T
0.5640701731993849	0.6378995307832876	0.2215466055606723	T	T	T
0.5648194798005506	0.8628051674557604	0.2354639518954718	T	T	T
0.2149421557703693	0.6697140435469801	0.3646625399360252	T	T	T
0.1457605005175012	0.6974136738147563	0.4216082508868842	T	T	T
0.9028596114430819	0.5953360616782238	0.3792692924888805	T	T	T
0.9304614220609733	0.8124193251195455	0.3625514004985664	T	T	T
0.3440846474052006	0.0492587483542173	0.3691480571215195	T	T	T
0.0351181394168794	0.2920769729791456	0.3910747538785154	T	T	T
0.1953986171529581	0.4034041295151238	0.3960819759112409	T	T	T
0.8264144510700504	0.0767174111812049	0.4347612080922706	T	T	T
0.5673957069309921	0.2782220539117313	0.3967244692445972	T	T	T
0.6901141400035760	0.0694642222099701	0.3739615867163633	T	T	T
0.3304081920912758	0.2577618963149812	0.2096152038152901	T	T	T
0.8437491143530810	0.1939866249409002	0.3085408292527225	T	T	T

Figure 3b State 3-Fe' (NUPDOWN=12)

1.0000000000000000					
8.7372206091223994	0.0000000000000000	0.0000000000000000			
0.0000000000000000	6.9809029500783426	0.0000000000000000			
0.0000000000000000	0.0000000000000000	25.0000000000000000			
K	Ni	O	H	Fe	
4	10	36	22	2	
Selective dynamics					
Direct					
0.0000000000000000	0.9295476953180497	0.0219900692777486	F	F	F
0.5000000000000000	0.8431778700801544	0.1149178963106294	F	F	F
0.9839322736665713	0.7635548654755738	0.2101506909694656	T	T	T
0.5720469578483806	0.6582625404154683	0.3434878537423067	T	T	T
0.0000000000000000	0.4295476953180497	0.0219900692777486	F	F	F
0.3336660000000009	0.4295476953180497	0.0219900692777486	F	F	F
0.6663339999999991	0.4295476953180497	0.0219900692777486	F	F	F
0.1663339999999991	0.3431778700801544	0.1149178963106294	F	F	F
0.5000000000000000	0.3431778700801544	0.1149178963106294	F	F	F
0.8336660000000009	0.3431778700801544	0.1149178963106294	F	F	F

0.9994611679687655	0.2650687297973300	0.2094269959464073	T	T	T
0.6686012805596754	0.2594037937934104	0.2099573810974764	T	T	T
0.1599366891808021	0.1844212505448989	0.3083382412773506	T	T	T
0.5043229393190756	0.1914013386109641	0.3068714561649004	T	T	T
0.1735150000000019	0.5955569454815901	0.0004884286588833	F	F	F
0.5000000000000000	0.5859389052830437	0.0000000000000000	F	F	F
0.8264849999999981	0.5955569454815901	0.0004884286588833	F	F	F
0.1735150000000019	0.2635384451545022	0.0434917098966210	F	F	F
0.5000000000000000	0.2731564853530557	0.0439801385555043	F	F	F
0.8264849999999981	0.2635384451545022	0.0434917098966210	F	F	F
0.0000000000000000	0.4995690800451484	0.0929278270328737	F	F	F
0.3264849999999981	0.5091871202437019	0.0934162556917641	F	F	F
0.6735150000000019	0.5091871202437019	0.0934162556917641	F	F	F
0.0000000000000000	0.1867866601151604	0.1369079655883780	F	F	F
0.3264849999999981	0.1771686199166140	0.1364195369294947	F	F	F
0.6735150000000019	0.1771686199166140	0.1364195369294947	F	F	F
0.1670188068726014	0.4204606286686434	0.1877390845509741	T	T	T
0.4994183404401985	0.4137047609218906	0.1872963474977535	T	T	T
0.8313418892246585	0.4203431829494593	0.1866885462808287	T	T	T
0.1677352584733240	0.1052489306964019	0.2306860868758052	T	T	T
0.5012769043746899	0.0997147734856887	0.2340405577702470	T	T	T
0.8349233749515498	0.1068039556159153	0.2329241502996869	T	T	T
0.9887519484494502	0.3540175551582297	0.2810649841738219	T	T	T
0.3424843470068929	0.3459979011721062	0.2802244823178757	T	T	T
0.6686829456944821	0.3436454724417793	0.2822687931193187	T	T	T
0.9804823556864120	0.0177564335293017	0.3253857094413460	T	T	T
0.3455240215051242	0.0196941662454118	0.3292256478573757	T	T	T
0.6697453282767182	0.0295469941257281	0.3294884557595122	T	T	T
0.3436370000000011	0.9295476953180497	0.0219900692777486	F	F	F
0.6563629999999989	0.9295476953180497	0.0219900692777486	F	F	F
0.1563629999999989	0.8431778700801544	0.1149178963106294	F	F	F
0.8436370000000011	0.8431778700801544	0.1149178963106294	F	F	F
0.2027656833030423	0.6931437859282019	0.2966994816127848	T	T	T
0.6153046783153033	0.7379985511216558	0.2376171004025172	T	T	T
0.2427535024227239	0.6535634788145862	0.4027778773821089	T	T	T
0.8652190860410380	0.7438606257814629	0.3932452608710719	T	T	T
0.4888441694526098	0.3033831307026463	0.3743141773333301	T	T	T
0.8488446843456385	0.3142043324013038	0.3754340051727137	T	T	T
0.1533006196227252	0.2816670689696755	0.3870313640687099	T	T	T
0.7959278397643194	0.1894151027836323	0.4188782697597532	T	T	T
0.2777910000000006	0.8194148176612188	0.0136009167645312	F	F	F
0.2777910000000006	0.0396805729748735	0.0303792217909731	F	F	F
0.7222089999999994	0.8194148176612188	0.0136009167645312	F	F	F
0.7222089999999994	0.0396805729748735	0.0303792217909731	F	F	F
0.2222089999999994	0.7330449924233307	0.1065287437974050	F	F	F
0.2222089999999994	0.9533107477369782	0.1233070488238468	F	F	F
0.7777910000000006	0.7330449924233307	0.1065287437974050	F	F	F
0.7777910000000006	0.9533107477369782	0.1233070488238468	F	F	F
0.2652393021710733	0.5811016677795160	0.2856638320368664	T	T	T
0.2683258726374935	0.8084682574444433	0.2970387295789275	T	T	T
0.5603623862044083	0.6352390178971795	0.2184802637140643	T	T	T
0.5603224207126388	0.8609255731127478	0.2333430735969828	T	T	T
0.2113863275339503	0.6786746742283700	0.3646607882165802	T	T	T
0.1637575134979643	0.7135148551061047	0.4246723270720282	T	T	T
0.8846789993575955	0.6067293747777507	0.3883678371490472	T	T	T
0.9161384776522645	0.8124664591114532	0.3632829682018043	T	T	T
0.3442135035633006	0.0423285190431237	0.3680699267323410	T	T	T
0.0418279479761864	0.3126754503018949	0.3887116029537534	T	T	T
0.2075114076810750	0.4046267928656428	0.3952514059756739	T	T	T
0.8763614787438263	0.0899852049649271	0.4206620591605397	T	T	T
0.5810817694164224	0.2753710069283667	0.3951342274108983	T	T	T

0.6800404624097232	0.0437293653355678	0.3687480761446141	T	T	T
0.3305002183363199	0.2545278489863937	0.2100256549352770	T	T	T
0.8452709607291959	0.1898292847239778	0.3062749035989010	T	T	T

Figure 3b State 4 (NUPDOWN=11)

```

1.000000000000000
8.7372206091223994      0.0000000000000000      0.0000000000000000
0.0000000000000000      6.9809029500783426      0.0000000000000000
0.0000000000000000      0.0000000000000000      25.0000000000000000
K      Ni      O      H      Fe
4      10      36      21      2
Selective dynamics
Direct
0.0000000000000000      0.9295476953180497      0.0219900692777486      F      F      F
0.5000000000000000      0.8431778700801544      0.1149178963106294      F      F      F
0.9855657382295325      0.7614201029244284      0.2115389249103933      T      T      T
0.5977774398584127      0.6759443418009170      0.3515305793151688      T      T      T
0.0000000000000000      0.4295476953180497      0.0219900692777486      F      F      F
0.3336660000000009      0.4295476953180497      0.0219900692777486      F      F      F
0.6663339999999991      0.4295476953180497      0.0219900692777486      F      F      F
0.1663339999999991      0.3431778700801544      0.1149178963106294      F      F      F
0.5000000000000000      0.3431778700801544      0.1149178963106294      F      F      F
0.8336660000000009      0.3431778700801544      0.1149178963106294      F      F      F
-0.0001457212074932      0.2624577821317718      0.2097277181870631      T      T      T
0.6687069035612215      0.2599816909140001      0.2098459580429816      T      T      T
0.1627403643398837      0.1805609600233550      0.3074839093943230      T      T      T
0.5102405203330357      0.1865072569457550      0.3064940627616792      T      T      T
0.1735150000000019      0.5955569454815901      0.0004884286588833      F      F      F
0.5000000000000000      0.5859389052830437      0.0000000000000000      F      F      F
0.8264849999999981      0.5955569454815901      0.0004884286588833      F      F      F
0.1735150000000019      0.2635384451545022      0.0434917098966210      F      F      F
0.5000000000000000      0.2731564853530557      0.0439801385555043      F      F      F
0.8264849999999981      0.2635384451545022      0.0434917098966210      F      F      F
0.0000000000000000      0.4995690800451484      0.0929278270328737      F      F      F
0.3264849999999981      0.5091871202437019      0.0934162556917641      F      F      F
0.6735150000000019      0.5091871202437019      0.0934162556917641      F      F      F
0.0000000000000000      0.1867866601151604      0.1369079655883780      F      F      F
0.3264849999999981      0.1771686199166140      0.1364195369294947      F      F      F
0.6735150000000019      0.1771686199166140      0.1364195369294947      F      F      F
0.1667377731765972      0.4188656587163943      0.1877164335487666      T      T      T
0.5003922047184920      0.4159338969233111      0.1878089453082538      T      T      T
0.8324418704104225      0.4198221041161350      0.1869419311753457      T      T      T
0.1655893175606754      0.1017780053924587      0.2289634166807286      T      T      T
0.5034853559508196      0.0998808866752149      0.2318397796180947      T      T      T
0.8345401173742497      0.1058299490548762      0.2328560675780531      T      T      T
-0.0075745568461527      0.3482796962610790      0.2801964269765673      T      T      T
0.3412249884445904      0.3397977774542585      0.2803740101037064      T      T      T
0.6672799930528849      0.3461581287105717      0.2815976223292857      T      T      T
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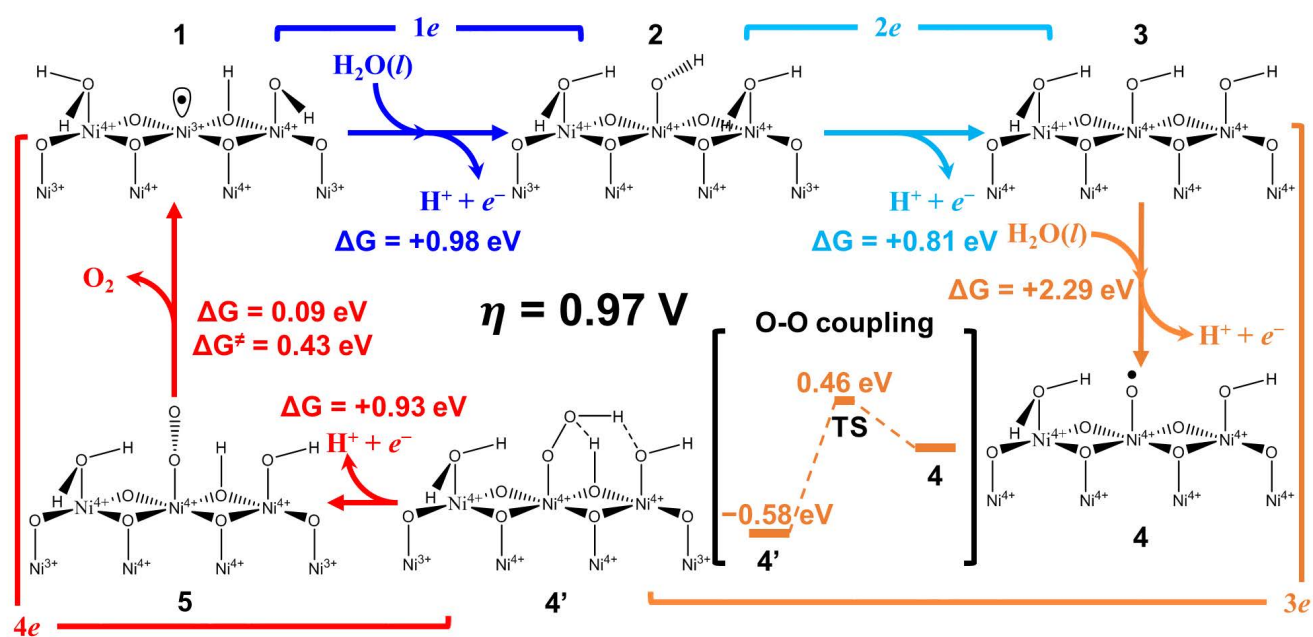
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Figure 3b State 5 (NUPDOWN=12)

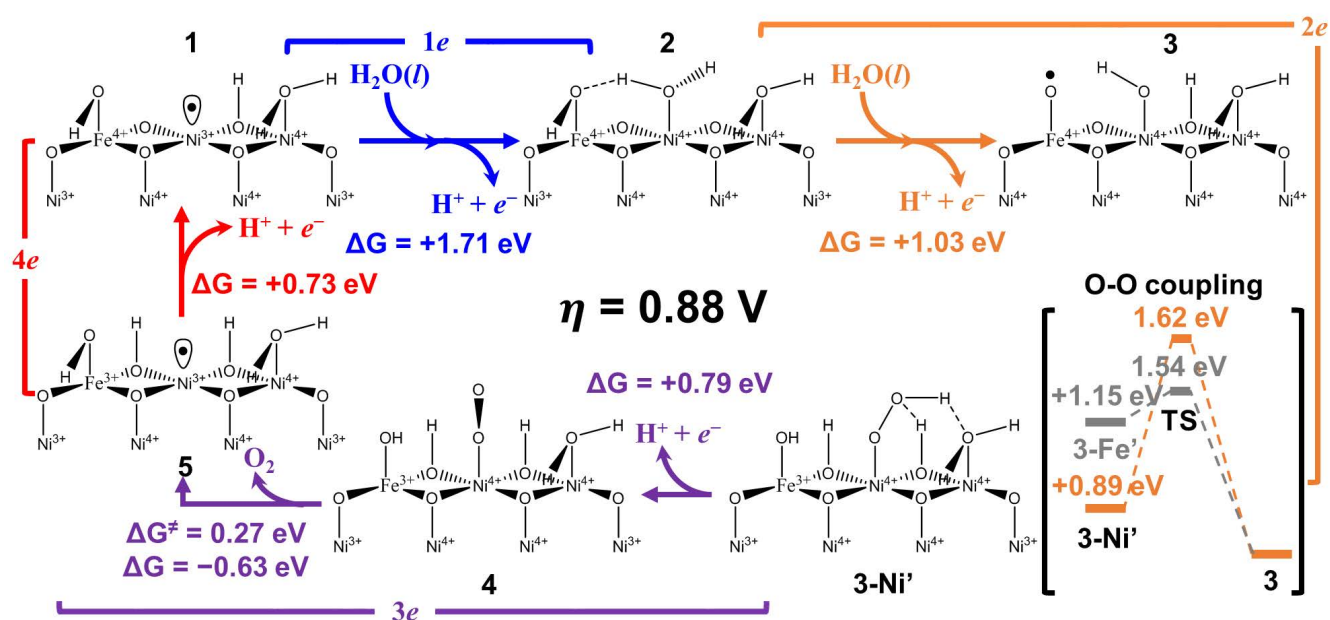
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Direct					
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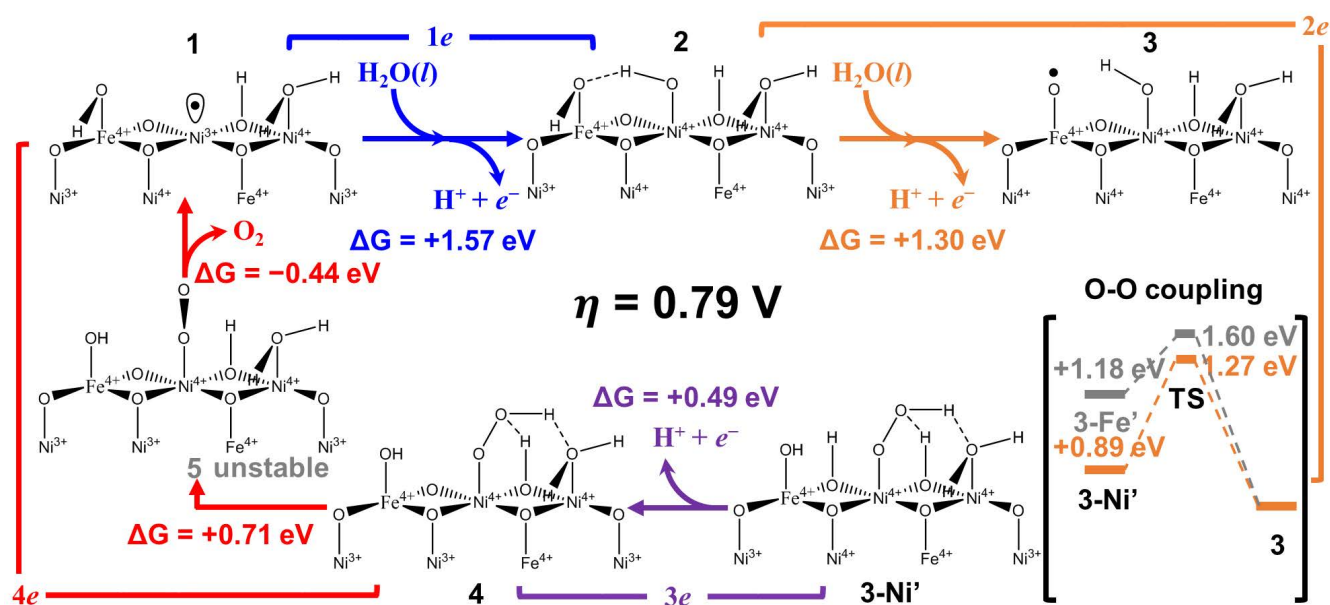
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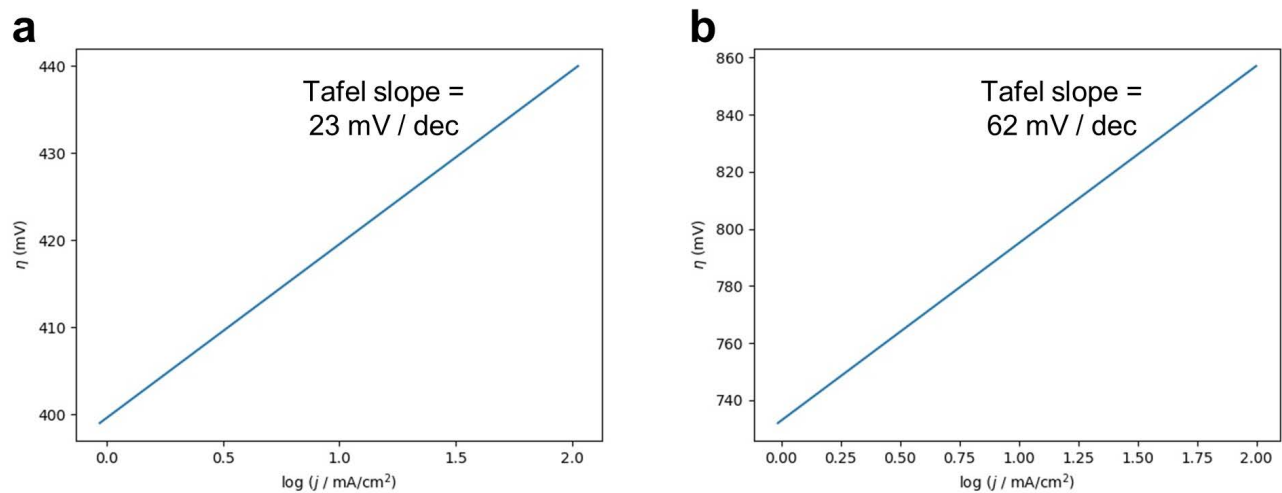
**Fig. S1.** The mechanistic cycle of OER catalyzed by pure  $\gamma$ -NiOOH surface with PBE predicted free energy differences  $\Delta G$  and barriers  $\Delta G^\ddagger$  at  $U = 2.10 \text{ V}$  ( $\eta = 0.97 \text{ V}$ ) corresponding to  $j = 10 \text{ mA/cm}^2$ .



**Fig. S2.** The mechanistic cycle of OER catalyzed by  $\gamma$ -NiOOH surface with 1/3 surface Fe doping with PBE predicted free energy differences  $\Delta G$  and barriers  $\Delta G^\ddagger$  at  $U = 2.01 \text{ V}$  ( $\eta = 0.88 \text{ V}$ ) corresponding to  $j = 10 \text{ mA/cm}^2$ .



**Fig. S3.** The mechanistic cycle of OER catalyzed by  $\gamma$ -NiOOH surface with 1/3 surface Fe doping plus 1/3 subsurface Fe doping with PBE predicted free energy differences  $\Delta G$  and barriers  $\Delta G^\ddagger$  at  $U = 1.92 \text{ V}$  ( $\eta = 0.79 \text{ V}$ ) corresponding to  $j = 10 \text{ mA/cm}^2$ .



**Fig. S4.** The Tafel plots for the case with 1/3 Fe on the top surface and 1/3 Fe at the subsurface layer, predicted by (a) B3PW91 and (b) PBE, respectively.

**Table S1.** Reaction free energies ( $\Delta G$ ) and barriers ( $\Delta G^\ddagger$ , denoted by TS) for OER elementary steps on pure  $\gamma$ -NiOOH predicted by B3PW91, including the explicit constant  $\mu_e$  correction and the dependence of applied electrochemical potential  $U$  (referenced to SHE). Note that the states 1 to 5 are corresponding to those in Figure 2.

Step	$\Delta G / \Delta G^\ddagger$ (eV)
<b>1 <math>\rightarrow</math> 2</b>	$2.0328 - 0.0798 \times U$
<b>2 <math>\rightarrow</math> 3</b>	$1.1483 + 0.1758 \times U$
<b>3 <math>\rightarrow</math> 4</b>	$2.3763 + 0.0274 \times U$
<b>4 <math>\rightarrow</math> 4' (TS)</b>	$0.5613 - 0.0354 \times U$
<b>4 <math>\rightarrow</math> 4'</b>	$-0.6947 - 0.1724 \times U$
<b>4' <math>\rightarrow</math> 5</b>	$0.8947 + 0.0013 \times U$
<b>5 <math>\rightarrow</math> 1 (TS)</b>	No barrier
<b>5 <math>\rightarrow</math> 1</b>	$-1.4983 + 0.0478 \times U$



**Table S2.** Reaction free energies ( $\Delta G$ ) and barriers ( $\Delta G^\ddagger$ , denoted by TS) for OER elementary steps on  $\gamma$ -NiOOH with 1/3 surface Fe doping predicted by B3PW91, including the explicit constant  $\mu_e$  correction and the dependence of applied electrochemical potential  $U$  (referenced to SHE). Note that the states 1 to 5 are corresponding to those in Figure 3a.

Step	$\Delta G / \Delta G^\ddagger$ (eV)
<b>1 <math>\rightarrow</math> 2</b>	$1.9279 + 0.0675 \times U$
<b>2 <math>\rightarrow</math> 3</b>	$1.8876 + 0.0515 \times U$
<b>3 <math>\rightarrow</math> 3-Ni' (TS)</b>	$0.4175 - 0.0258 \times U$
<b>3 <math>\rightarrow</math> 3-Ni'</b>	$-0.2465 - 0.0777 \times U$
<b>3 <math>\rightarrow</math> 3-Fe' (TS)</b>	$1.5689 - 0.0113 \times U$
<b>3 <math>\rightarrow</math> 3-Fe'</b>	$0.3370 - 0.1166 \times U$
<b>3-Ni' <math>\rightarrow</math> 4</b>	$1.1312 + 0.0400 \times U$
<b>4 <math>\rightarrow</math> 5 (TS)</b>	No barrier
<b>4 <math>\rightarrow</math> 5</b>	$-1.6151 - 0.2557 \times U$
<b>5 <math>\rightarrow</math> 1</b>	$1.1721 + 0.1743 \times U$

Table S3. Reaction free energies ( $\Delta G$ ) and barriers ( $\Delta G^\ddagger$ , denoted by TS) for OER elementary steps on  $\gamma$ -NiOOH with 1/3 surface Fe doping plus 1/3 subsurface Fe doping predicted by B3PW91, including the explicit constant  $\mu_e$  correction and the dependence of applied electrochemical potential  $U$  (referenced to SHE). Note that the states 1 to 5 are corresponding to those in Figure 3b.

Step	$\Delta G / \Delta G^\ddagger$ (eV)
<b>1 <math>\rightarrow</math> 2</b>	$2.0054 + 0.0227 \times U$
<b>2 <math>\rightarrow</math> 3</b>	$1.2532 - 0.0345 \times U$
<b>3 <math>\rightarrow</math> 3-Ni' (TS)</b>	$0.5141 + 0.0818 \times U$
<b>3 <math>\rightarrow</math> 3-Ni'</b>	$-0.1806 - 0.0342 \times U$
<b>3 <math>\rightarrow</math> 3-Fe' (TS)</b>	$0.4778 + 0.1212 \times U$
<b>3 <math>\rightarrow</math> 3-Fe'</b>	$0.6966 - 0.0631 \times U$
<b>3-Ni' <math>\rightarrow</math> 4</b>	$1.3149 + 0.1402 \times U$
<b>4 <math>\rightarrow</math> 5</b>	$0.6125 - 0.0139 \times U$
<b>5 <math>\rightarrow</math> 1 (TS)</b>	$0.1658 - 0.0140 \times U$
<b>5 <math>\rightarrow</math> 1</b>	$-0.7467 - 0.0803 \times U$

**Table S4. Comparison of predicted  $\eta$ 's for OER on (Ni,Fe)OOH catalysts.**

Methods	$\eta$ (V) at 10 mA/cm <sup>2</sup> for different surface Fe concentration C[Fe <sub>s</sub> ] and below surface (considered as bulk) Fe concentration C[Fe <sub>b</sub> ]		
	C[Fe <sub>s</sub> ] = 0, C[Fe <sub>b</sub> ] = 0	C[Fe <sub>s</sub> ] = 1/3, C[Fe <sub>b</sub> ] = 0	C[Fe <sub>s</sub> ] = 1/3, C[Fe <sub>b</sub> ] = 1/9*
<b>Expt.</b>	0.7 (Ref. (24))		0.3-0.4 (Ref. (24–26))
<b>B3PW91</b>	1.22	0.83	0.42
<b>PBE0</b>	1.16	—	0.61
<b>PBE</b>	0.97	0.88	0.79

\* Note that here the 1/3 subsurface Fe doping is converted to C[Fe<sub>b</sub>] by including the bottom two pure Ni layers, which might not correspond to the realistic C[Fe<sub>b</sub>], as the deeper bulk region (beyond the four layer slab model we considered) might contain more Fe doping.

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